DESIGN AND SYNTHESIS OF HEAT EXCHANGER NETWORKS WITH VARIABLE STREAM PROPERTIES

BY

FAYSAL MOHAMMAD AL-KHULAIFI

A Thesis Presented to the
DEANSHIP OF GRADUATE STUDIES

KING FAHD UNIVERSITY OF PETROLEUM & MINERALS

DHAHRAN, SAUDI ARABIA

In Partial Fulfillment of the
Requirements for the Degree of

MASTER OF SCIENCE

In

CHEMICAL ENGINEERING

MAY, 2014

DESIGN AND SYNTHESIS OF HEAT EXCHANGER NETWORKS WITH VARIABLE STREAM PROPERTIES

Faysal Al Khulaifi

CHEMICAL ENGINEERING DEPARTMENT

May 2014

KING FAHD UNIVERSITY OF PETROLEUM & MINERALS

DHAHRAN- 31261, SAUDI ARABIA

DEANSHIP OF GRADUATE STUDIES

This thesis, written by **FAYSAL MOHAMMAD AL KHULAIFI** under the direction of his thesis advisor and approved by his thesis committee, has been presented and accepted by the Dean of Graduate Studies, in partial fulfillment of the requirements for the degree of **MASTER OF SCIENCE IN CHEMICAL ENGINEERING.**

Ealmtain

Dr. Eid M. Al-Mutairi
(Advisor)

Dr. Mohammed Ba-Shammakh
Department Chairman

B.H.

Dr. Housam Binous
(Member)

Dr. Salam A. Zummo
Dean of Graduate Studies

Dr. Naim M. Faqir
(Member)

2|12|14

Date

Dedication

TO MY BELOVED PARENTS

MOHAMMAD AL-KHULAIFI

&

MODHI AL-OJAIMI

TO MY DEAR BROTHERS AND SISTERS

FADWA, MANSOUR, YOUSEF, DANIA & ABDULLAH

ACKNOWLEDGMENTS

I would like to thank KFUPM for providing me the resources and opportunity to conduct my research and continue my education.

I would like to express my deep gratitude and profound appreciation to my advisor, Dr. Eid M. Al-Mutairi, for his total cooperation, help, encouragement and supervision during the research work.

Appreciations and thanks to Dr. Housam Binous and Dr. Naim Faqir for their excellent cooperation and advice during this endeavor.

I would like to thank king Abdulaziz city for science and technology (KACST) and their National science, technology and innovation plan (NSTIP) for funding and supporting this research work under project No. 09-ENE756-04.

Special thanks to the faculty, staff and graduate students of Chemical Engineering department for all the help and cooperation.

I would like to express gratitude to my parents, my brothers and sisters for their support, encouragement and kindness.

TABLE OF CONTENTS

LIST OF TABLES

LIST OF FIGURES

LIST OF ABBREVIATIONS

HEN	:	Heat Exchanger Network
TAC	:	Total Annual Cost
TIC	:	Total Investment Cost
LP	:	Linear Programming
NLP	:	Non-Linear Programming
MILP	:	Mixed Integer Linear Programming
MINLP	:	Mixed Integer Non-Linear Programming
PTP	:	Process-to-Process
HENS	:	Heat Exchanger Network Synthesis
EMAT	:	Exchanger Minimum Approach Temperature

ABSTRACT

Full Name : Faysal Mohammad Al Khulaifi

Thesis Title : Design and Synthesis of Heat Exchanger Networks With Variable Stream Properties.

Major Field : Master of Science in Chemical Engineering

Date of Degree : May 2014

In recent years, demands for highly efficient processes have grown substantially due to environmental concerns, increase in global demand for high-quality products and search for more cost-effective ways to maintain operational goals. For more than 30 years, research in the field of process optimization has brought us closer to achieving rigorous mathematical models that can best describe an efficient, reliable heat exchange network for a process in order to reduce utility and resource costs while improving returns on investments. In this work, mathematical HEN models were designed to consider flexibility of operational conditions, such as temperature and flow rate, to reach an optimized process. This was done by proposing a novel approach to modeling that will investigate the effects of stream property profiles when considered as a variable function of temperature. The minimum total annual cost in two case studies has changed in the range of -0.9% to 7.2% compared to base cases (where properties are assumed constant). It was also observed that investment costs are mostly affected by heat exchanger design variables (heat transfer coefficient, viscosity and thermal conductivity) while utility costs are mostly affected by variable heat capacity.

ملخص الرسالة

الاسم الكامل: فيصل محمد الخليفي

عنوان الرسالة: تصميم و تركيب شبكات تبادل حراري ذات خصائص تدفق متغيرة.

التخصص: ماجستير العلوم في الهندسة الكيميائية.

تاريخ الدرجة العلمية: مايو 2014

في السنوات الأخيرة ، نمت المطالب للعمليات الصناعية ذات الكفاءة العالية إلى حد كبير بسبب المخاوف البيئية ، و الزيادة في الطلب العالمي على منتجات عالية الجودة ، بالإضافة إلى البحث عن طرق أكثر فعالية من حيث تقليل التكاليف مع الحفاظ على الأهداف التشغيلية. لأكثر من 30 سنة ، قامت الأبحاث في مجال الحلول المثلى بتحقيق نماذج رياضية صارمة قادرة على إيجاد شبكات مبادلات حرارية في المعامل الصناعية ذات كفاءة و اعتمادية عالية و ذلك للتقليل من تكاليف مرافق التبريد و التسخين و غيرها من المصادر مع تحسين العوائد على الإستثمارات. في هذا البحث ، تم تصميم نماذج رياضية تصف شبكات مبادلات حرارية تأخذ بعين الاعتبار المرونة في حالات التشغيل ، مثل تغيرات درجة الحرارة و معدل التدفق ، و ذلك للتوصل إلى عملية صناعية مثلى. و قد تم ذلك من خلال اقتراح طريقة جديدة لنماذج رياضية من شأنها التحقق من تأثير السعة الحرارية للمواد على أية عملية صناعية عند اعتبارها دالة متغيرة مع درجة الحرارة بعكس ما هو حاصل في أبحاث سابقة في هذا المجال. تم ملاحظة تغير في التكلفة السنوية ما بين حالتين دراسيتين يقدر بنسبة 0.9-% إلى 7.2% مقارنة بالحالات الأساسية (حيث لا يوجد تغيرات في خصائص التدفق). كما لوحظ ان التكاليف اللإستثمارية تتأثر بشكل كبير بمتغيرات تصميم المبادل الحراري مثل (معامل التبادل الحراري ، اللزوجة و الموصلية الحرارية) ، بينما تكاليف المنافع تتأثر بشكل أكبر بالسعة الحرارية المتغيرة.

CHAPTER 1

INTRODUCTION

In recent years, demands for highly efficient processes have grown substantially due to environmental concerns, increase in global demand for high-quality products and search for more cost-effective ways to maintain operational goals. For more than three decades, research in the field of process optimization has brought us closer to achieving rigorous mathematical models that can best describe an efficient, reliable heat exchanger network (HEN) for a process in order to reduce utility and resource costs while improving returns on investments. Striving to improve the tools of HEN optimization can move us closer to reaching those goals.

This work investigates the effects of considering stream property profiles on the optimization of HENs for two case studies. This is done by proposing a mathematical formulation that takes into consideration the variability of properties such as heat capacity and viscosity with temperature. These efforts will lead to a more accurate and representative optimum HENs that correlate more closely with actual, real process.

An introductory chapter will present the basics of optimization and the objectives of this research. Then, a chapter on literature review will cover a number of prominent works in the field of optimization. Next, the effects of varying heat capacity with temperature on the optimality of HENs will be discussed thoroughly in chapter 3. Finally, we introduce variability to more properties, such as viscosity and thermal conductivity, and observe its impact on the optimum HEN.

1.1 Types of Optimization Approaches

There are two types of optimization approaches that are widely used in literature. Sequential optimization is one approach, which involves the synthesis of HENs as a sequence of problems. The sequence starts with the problem of determining minimum utility usage. Then, the minimum number of heat exchangers is established. Finally, an optimization problem involving the minimization of total investment cost (TIC) or total annual cost (TAC) with fewest heat exchangers is solved. Graphical methods and pinch technology are examples of this approach to optimization. The shortcomings of this approach include suboptimal solutions and the exclusion of trade-offs for a variety of factors impacting TAC [1-3].

The other approach is called the simultaneous optimization, which involves the synthesis of optimum HENs using a mathematical program that optimizes the process. The program, or model, includes an objective function that describes the costs associated with the HEN subject to a set of constraints. The optimization is done by proposing a superstructure that represents all potential configurations that the HEN could take. The decisions to determine the most optimum solution, based on models, are done in a simultaneous and integrated manner [7, 8].

The complex nature of the mathematical models in addition to the computational power required to solve them can be considered as a disadvantage of the simultaneous approach [7, 8]. However, this is becoming less of a concern nowadays due to the continuous advancement in computer technology and the proliferation of software packages that help in solving these optimization models.

The mathematical model formulation can have different outcomes based on the linearity of the model and the inclusion of binary integers as logical constraints. If the formulation involves a linear objective function and linear constraints, then the result is a Linear Programming (LP) model. Conversely, any non-linearity in the objective function or the constraints creates a Non-Linear Programming (NLP) model. Finally, if binary (or mixed) integers were used as logical constraints in the formulation, a mixed integer program is produced. Thus, we could have a Mixed Integer Linear Program (MILP) or a Mixed Integer Non-Linear Program (MINLP) formulation based on the aforementioned criteria. The work proposed in this paper will utilize MINLP in the synthesis of HENs with variable stream physical properties [1-3, 23, 28].

1.2 Scope and Objectives

The goal of this work is to utilize the simultaneous approach for the design of mathematical HEN models that consider flexibility of operational conditions, particularly temperature, to reach an optimum solution. Most of the previous works in HEN optimization were based on stringent observation of the pinch design method or the simultaneous approach, in which most process stream properties were assumed constant. In this work, a new approach which will allow more flexibility in the heat exchanger network design is to be developed. A novel mathematical modeling approach will be proposed to investigate effects of stream properties like heat capacity, viscosity and heat transfer coefficient when they are considered as variable functions of temperature in the

HEN. Success in this approach will positively impact the accuracy of the optimum HEN and enhance its conformity with real industrial applications.

Since mathematical formulations in process optimization contain energy balances and heat exchanger design considerations, it is expected that the aforementioned properties will have a significant impact on the optimum HEN. The impact will manifest in the form of either significant changes to energy loads within the superstructure of the process, or in the form of alterations to the process matches found in certain networks. These considerations provide the plan to pursue our objectives.

Thus, the objectives of this research can be defined as follows:

- Develop a mathematical formulation that reliably predicts the optimum HEN for given process operation conditions.
- Introduce the effects of stream property profiles under variable temperatures to the mathematical formulation.
- Investigate the impact of variable stream properties on the optimum HEN compared to the base case (where stream properties are constant).
- Apply the formulation on appropriate case studies.

CHAPTER 2

LITERATURE REVIEW

Mathematical programming techniques have been effectively used to address several important categories of HENs [10, 11]. In an attempt to exploit the interactions between the process operating conditions (i.e. stream temperatures and flow rates) and the heat recovery network, Papoulias and Grossmann (1983) developed a strategy for simultaneous optimization of the process and heat integration based on mixed integer linear programming (MILP) [1-3]. This approach allows the flow rates to vary in order to optimize the process and the associated network of heat exchangers. In order to avoid nonlinear terms in the formulation, fixed temperature intervals are defined.

Duran and Grossmann (1986) introduced a mathematical approach to the optimization of heat exchange networks where the supply and target temperatures are allowed to vary [4]. Mathematical constraints were introduced to account for the unknown temperature and to locate candidate and true pinch points, thereby ensuring that the final flowsheet will feature the minimum utility target. According to this approach, bounds on the energy requirements of the process are explicitly included within the synthesis problem. However, the structure and overall cost of the heat recovery system are not traded off with process costs.

Pistikopoulos and Grossmann (1989) developed metrics for measuring the flexibility of a heat exchanger network. Their method allows for the identification of flexibility levels that maximize expected profits in retrofitting designs through nonlinear models. [9].

Yee et al. (1990) proposed a structural optimization model, where process alternatives are optimized simultaneously with the heat exchanger network that accommodates the heating and cooling requirements of the process streams [6-8]. They introduced a superstructure representation which included many possible flowsheet alternatives. However, the number of variables and constraints that are needed to produce the required mathematical representations may be large. Thus, simplifying assumptions may be required.

Grossmann *et al.* (1998) developed another method for the simultaneous optimization of flowsheet and heat integration. It is based on introducing integer variables that give a general formulation for heat loads and composite curves [5].

Papalexandri and Pistikopoulos (1998) presented a generic superstructure of heat integration alternatives to investigate interactions between process operating conditions, namely temperature and flowrates, and the heat recovery network. The superstructure was utilized to allow the optimization of process alternatives and heat recovery within one problem based on total annual cost (TAC) [17].

Zhang and Zhu (2000) developed a network pinch for HEN retrofit considering changes in the process parameters, mainly, temperature changes and flow rates. In their work, simultaneous approach for HEN retrofit is considered where process models are developed followed by investigating the variation of flow rates and temperatures of process streams and predict the impact of these changes on a HEN [16].

More recent work on flexibility of HEN where uncertainty is introduced because of variable flow rates and temperatures was investigated by Chen and Hung (2004, 2007) [13, 14]. They presented a novel strategy for the synthesis of cost-effective flexible heat-exchange networks (HENs) that involve specific uncertainty for source temperatures and flowrates. They used a decomposition method to reduce the complexity of the problem.

Recently, Hasan *et al.* (2009a, 2009b) proposed extending HEN synthesis to systems involving multi-stream exchangers and non-isothermal phase changes. They developed novel MINLP formulations and algorithms, but did not consider the property variations or flexibility considerations [29].

There are also other attempts to include other effects on HEN design in the optimal design for the process and HEN. For instance, Adonyi *et al.* (2003) work on integrating the heat integration and scheduling in batch processes to determine a solution that requires minimal utility and satisfies a constraint on the makespan [18]. However, this integration considered fixed supply and target temperatures.

Recently, Al-Mutairi and El-Halwagi (2009) extended that to continuous processes where scheduling considerations are incorporated at the design stage of HENs. They developed an integration method that integrates process operation schedules and HEN design [19].

Due to the need for optimization of HENs operating at different periods, the concept of multi-period HENs was introduced by researchers in this field. To elaborate, a multi-period HEN is defined as a network which is subject to parameter changes that arise from routine process procedures, such as initiating or terminating an operation, or as a result of known changes in demand, such as winter and summer operations.

To this effect, the summer and winter operations could be designated as period 1 and 2, respectively [28]. Verheyen and Zhang (2006) developed a systematic methodology for the design of multi-period HENs based on a suitable single period model which is both accurate with reasonable solving times [20]. Other work related to HEN optimal design in general discussed incorporation of the options of merging and/or splitting process streams from multiple origins in heat exchanger network (HEN) design. The utility and capital costs of a traditional HEN may both be reduced significantly by this procedure [21, 22].

As remarked earlier, most of the work involved cost optimality or energy conservation without considering aspects of operation such as flexibility, operability, etc. While several efforts since early 80s have considered HEN for multi-period operation, they all have neglected the variability of stream properties (e.g. viscosity, heat capacity) that can significantly affect the actual operation of a HEN. Thus, a methodology to consider optimality in the presence of operational flexibility and robustness with significant variations in stream properties is essential.

More recently, the work of Nejad *et al.* [27] involved the modification of a heat exchanger network design for an ammonia plant while investigating physical properties variation. In the paper, the authors use a sequential approach, particularly the pinch method, in order to reach an optimum HEN. They used stream segmentation in order to account for the variable physical properties within the hot and cold streams and compared their outcomes with the results of the optimization without segmentation.

In other work, Al-Mutairi and Odejobi [30] have investigated the effects of variable capacity flow rate on the optimization of HEN in a thermal power plant. This was done using an MINLP optimization model by comparing a base case with two cases involving the same thermal plant with a 5% increase and a 5% decrease in capacity flow rate, respectively. Their conclusions show significant changes to costs associated with the plant when variability was introduced.

The above literature review is more relevant to optimality and flexibility of HEN. However, Furman and Sahinidis [23] provided a critical review of the current state-of-the-art in HENs that provides a helpful look at the field of process optimization.

Most research in this field was done to investigate the effects of flexibility in stream conditions such as temperature and flow rate on the optimum HEN. It accounts for the uncertainty in real applications that arises from weather conditions, supply and demand, shut down and startup of processes, which are macro-level issues. However, very little research addresses the issue of variability in stream properties and how they impact process optimization. Thus, we will start by introducing heat capacity to a novel mathematical formulation and discuss the ramifications in chapter 3. Then, another chapter will address the effects of adding more stream property profiles such as viscosity and thermal conductivity into a more sophisticated formulation and how it affects the optimized HEN.

CHAPTER 3

OPTIMUM HEAT EXCHANGER NETWORKS WHILE CONSIDERING VARIABLE HEAT CAPACITY

This chapter will cover variability of heat capacity and its impact on the solution of optimum HEN. We start by defining heat capacity and how it relates to temperature in HENs. Then, the methodology to derive the model will be discussed. Afterwards, we present the problem statement and show the mathematical formulation to solve the problem in detail. Next, a description of the case studies in this research will be provided. Finally, results and discussions will be presented.

3.1 Heat Capacity

Heat capacity (C_p) can be defined as the energy required to raise the temperature of 1 unit of mass by 1 unit of temperature. Typical units of measurement are *kJ / kg K*. Naturally, heat capacity is a strong function of temperature. Values of heat capacity measured at 20^{o}C for different materials are widely used and tabulated in different resources and handbooks.

On the other hand, if we look at the literature of optimum HENs and how it treats heat capacity, it can only be found as part of a parameter in process streams called the capacity flow rate. This parameter is the result of multiplying the mass flow rate of a stream with the heat capacity of that stream. In various examples and case studies found in literature, this parameter is often assumed constant, which does not correlate with the fact that heat capacity varies with temperature inside the process.

We can create better tools to predict the optimum HEN for different processes by modifying commonly used mathematical formulations to include the effects of variable heat capacity. This will be further detailed in the next few sections.

3.2 Methodology

Mathematical programming is widely used for heat exchanger network synthesis. It is more broad and rigorous and has been the preference of most recent research in this area. The proposed HEN problem can be formulated as a mixed-integer nonlinear programming (MINLP) problem. This is due to nonlinearity arising from the inclusion of cost indices associated with heat exchanger area calculations, represented by new terms added to the objective function.

Approaches found in literature allowing for variable temperatures and flows (e.g., floating pinch method) result in MINLPs which don't take into consideration the changes in the feed or product properties. *Hence, we will develop models that account for changes in physical properties such as heat capacities, viscosities etc.* for this chapter, the focus will be on introducing heat capacity as a variable. This will be the first step in the investigation of variability across multiple physical properties. By taking this approach, we can easily identify any problems associated with model modifications and stamp them out before advancing into more sophisticated simulations that include more stream property profiles. Additionally, it makes it much easier to contrast the magnitude of the impact on the optimum HEN for different properties. The novel formulations and procedures developed in this work will necessarily involve highly combinatorial and complex MINLP, as discussed earlier, which could be challenging but important to pursue.

The mathematical formulation for this problem will utilize the work of Yee and Grossman (1990) as its basis. Their model will be modified to allow for the observation of variability in temperature and its effect on heat capacity. Ultimately, the purpose is to investigate the effect of these modifications on fixed and operational costs of the optimized HEN.

A few simplifying assumptions must be made in order to reach these goals. It is assumed that:

(1) There will only be one type of hot utility and cold utility (i.e. steam and water).
(2) Hot and cold utilities will be placed outside the superstructure that represents the HEN.
(3) The process involves isothermal-mixing only.
(4) Each stream contains pure, incompressible fluid species in the liquid phase.
(5) The heat exchangers in the superstructure have a double-pipe configuration.

The first two assumptions are part of the Yee and Grossman formulation, which is the basis for our modifications. The third assumption makes energy balances linear, which simplifies calculations. The fifth assumption corresponds to the design of the heat exchangers. Cold streams will flow in the inner tube while hot streams will flow in the outer pipe. Figure 3-1 illustrates this configuration.

In order to attempt the proposed problem, a number of software packages will be used. To solve for the optimum HEN considering variable physical properties, DICOPT will be utilized as a solver. It is a part of a larger software library known as GAMS, which is a well-known program designed as an optimizer software.

On the other hand, representation of case studies and their thermodynamics will require the use of ASPEN HYSYS. Thus, data for heat capacity versus temperature was obtained from HYSYS unless otherwise mentioned. The formulation and its application on case studies will be done on a computer equipped with an Intel® Core™ i7 – 2700K CPU at 3.50 GHz and 16 Gigabytes of RAM.

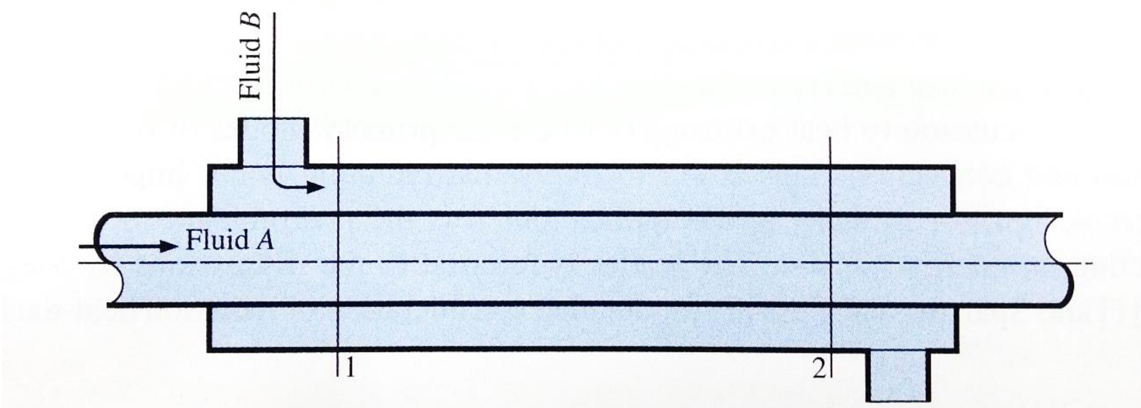

Figure 3-1: Schematic of a double-pipe heat exchanger [32].

3.3 Problem Statement

The Heat Exchanger Network Synthesis (HENS) problem to be attempted in this work can be stated as follows:

"Given a number of hot process stream, N_H, that needed to be cooled and a number, N_U, of cold process stream that needed to be heated. Supply temperature, Ts, and target temperature T_T, of each stream are also provided. Available for use are heating and cooling utilities, Q_{HU}, and Q_{CU}, respectively, whose costs, supply temperatures, and target temperatures are given. Also given are the stream mass flow rate (F) or volumetric flow rate (Q). The stream heat capacity C_p is defined as a function of stream interval and target temperatures. It is desired to synthesize an optimal and cost effective heat exchanger networks which can transfer heat from hot process streams and hot utilities to cold process stream and cold utilities for varying heat capacity."

The objective then is to design a flexible heat exchanger network which exhibits minimum TAC and optimum performance when subjected to variations in stream properties. It is intended to develop a superstructure involving two hot and two cold streams along with the hot and cold utilities, as demonstrated in figures 3-2 and 3-3. Ultimately, this approach will be applied in several case studies to observe its viability.

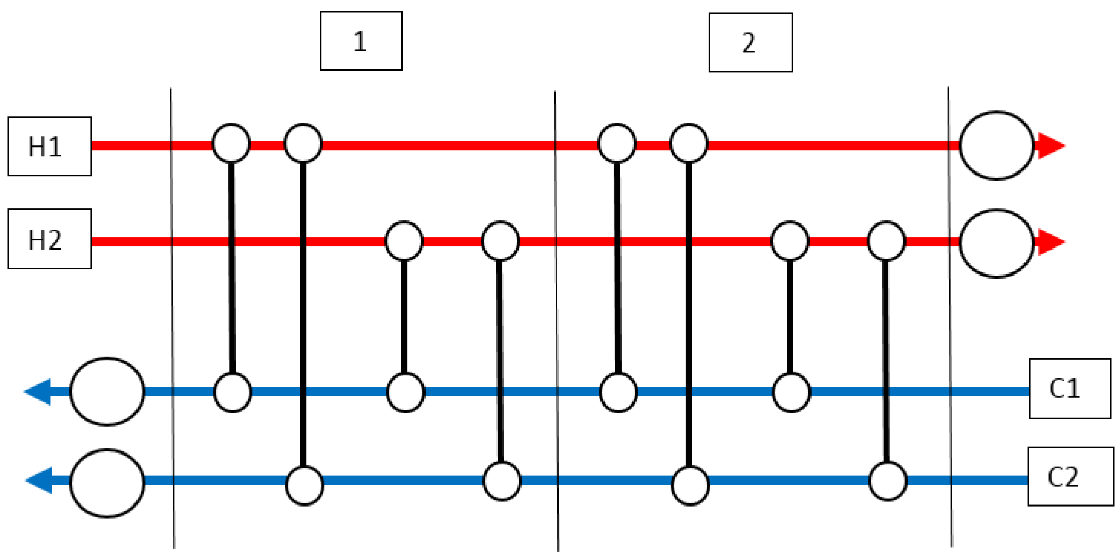

Figure 3-2: Grid representation of two hot and two cold streams.

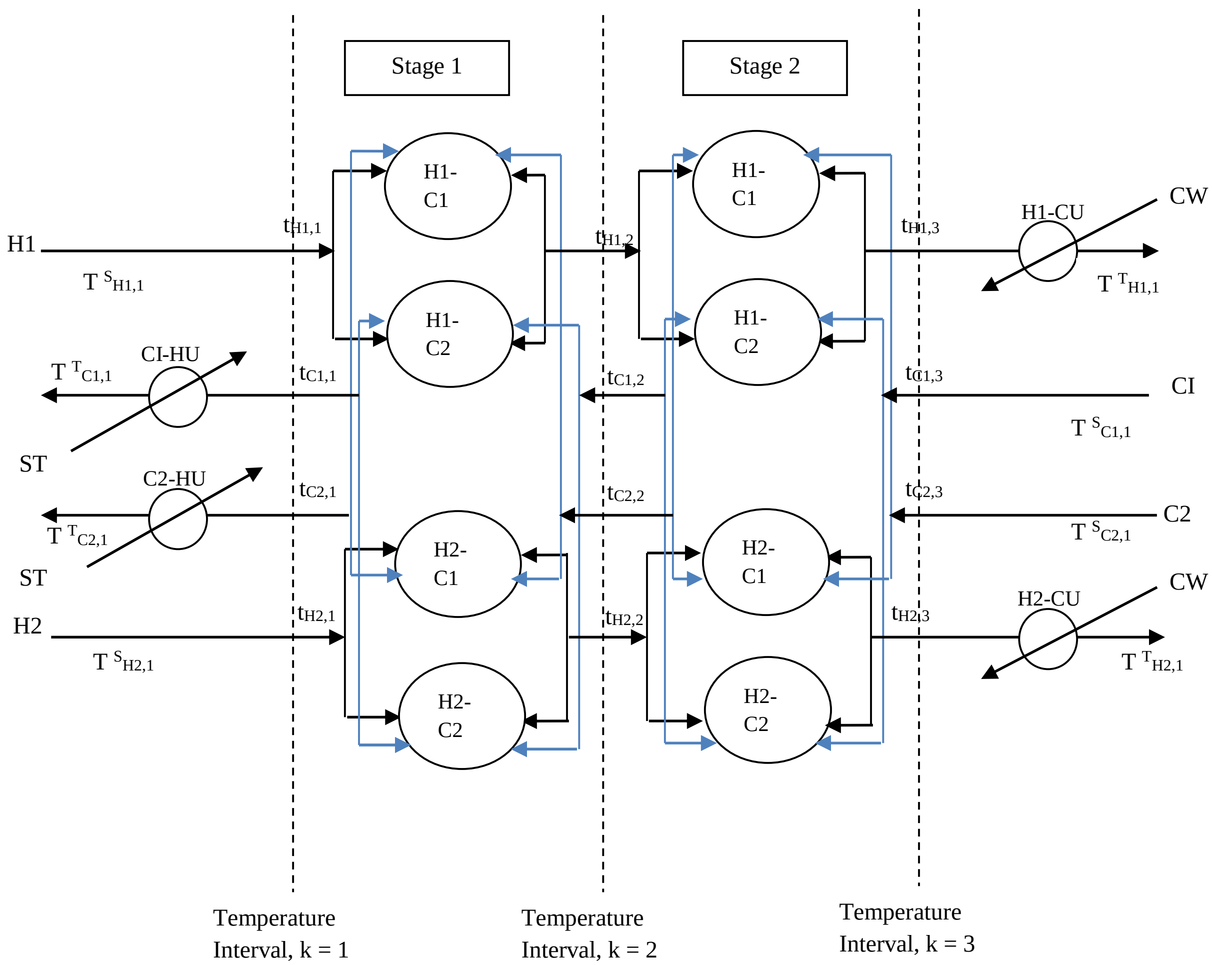

Figure 3-3: Two-stage superstructure

3.4 Mathematical Formulation

For this superstructure, the mathematical formulation will utilize and apply assumptions made previously in the methodology section. It should be noted that the supply temperature of H1 (Hot Stream 1) corresponds to location k = 1 in the superstructure, while its temperature in any other location is an optimized variable. This applies to interval and supply temperatures of other streams as displayed in figure 3-3.

Constraints

1. Overall energy balance for each stream:

   To certify enough heating and cooling is available to process streams, an overall heat balance is necessary. This constraint means that the overall heat transfer required in each stream is equivalent to the summation of heat exchanged with other streams at different stages of the superstructure added to utility exchanges with the streams:

$$\left(T_i^S C_{p,i}^S - T_i^T C_{p,i}^T\right) F_i = \sum_{k \in K} \sum_{j \in C} q_{ijk} + q_{i,CU} \qquad i \in H \tag{3-1}$$

$$\left(T_j^T C_{p,j}^T - T_j^S C_{p,j}^S\right) F_j = \sum_{k \in K} \sum_{i \in H} q_{ijk} + q_{HU,j} \qquad j \in C \tag{3-2}$$

2. Heat balance at each interval:

   This constraint is designed to find the optimum interval temperatures through stage energy balances. Thus, the heat balance for each interval is the following:

$$\left(t_{i,k} C_{p,i,k} - t_{i,k+1} C_{p,i,k+1}\right) F_i = \sum_{j \in C} q_{ijk} \qquad k \in K,\ i \in H \tag{3-3}$$

$$\left(t_{j,k} C_{p,j,k} - t_{j,k+1} C_{p,j,k+1}\right) F_j = \sum_{i \in C} q_{ijk} \qquad k \in K,\ j \in C \tag{3-4}$$

As noted earlier, $t_{i,k}$ and $t_{j,k}$ are variables to be optimized in the superstructure. Additionally, the set k = 1, …, NOK+1 is utilized to indicate temperature locations in the superstructure.

3. Assignment of superstructure inlet temperatures:

The supply temperatures for each stream in the superstructure are assumed to be the same as the inlet interval temperatures. For hot streams, this is exactly the temperature at k = 1. Conversely, the inlet superstructure temperature for cold stream is equal to temperature at k = NOK+1.

$$T_i^S = t_{i,1}, \qquad i \in H \qquad (3\text{-}5)$$

$$T_j^S = t_{j,NOK+1,} \qquad j \in C \qquad (3\text{-}6)$$

4. Temperatures feasibility:

Stream temperatures must decrease inside the superstructure from left to right. The interval temperature at the terminal stage might not be equal to the target temperature of the stream. This allows for the possibility to use utilities outside the superstructure.

$$t_{i,k} \geq t_{i,k+1} \qquad k \in K,\ i \in H \qquad (3\text{-}7)$$

$$t_{j,k} \geq t_{j,k+1} \qquad k \in K,\ j \in C \qquad (3\text{-}8)$$

$$T_i^T \leq t_{i,NOK+1} \qquad i \in H \qquad (3\text{-}9)$$

$$T_j^T \geq t_{j,1} \qquad j \in C \qquad (3\text{-}10)$$

5. <u>Energy balance for the hot and cold utility loads:</u>

To determine hot and cold utility loads in the superstructure, outlet temperatures at the last stage and target temperatures for process streams are utilized. This can be done using the following constraint:

$$\left(t_{i,NOK+1}C_{p,i,NOK+1} - T_i^T C_{p,i}^T\right)F_i = q_{i,CU} \qquad i \in H \tag{3-11}$$

$$\left(T_j^T C_{p,j}^T - t_{j,1}C_{p,j,1}\right)F_j = q_{HU,j} \qquad j \in C \tag{3-12}$$

6. <u>Logical constraints:</u>

A binary variable *z* can be defined to find out the presence of a process match (*i*,*j*) in a stage *k* or with available utility. Thus, a binary variable *z* is defined to have the values of either 0 or 1. This variable has the value '1' if a match exists in the optimum network. On the other hand, it has the value '0'. Thus, the following constraints are defined:

$$q_{ijk} - \Omega z_{ijk} \le 0, \qquad i \in H\ , j \in C\ , k \in K, \tag{3-13}$$

$$q_{i,CU} - \Omega z_{i,CU} \le 0, \qquad i \in H\ , \tag{3-14}$$

$$q_{HU,j} - \Omega z_{HU,j} \le 0, \qquad j \in C\ , \tag{3-15}$$

$$z_{ijk}\ ,\ z_{i,CU}\ ,\ z_{HU,j} = 0,1$$

7. <u>Heat exchanger area calculation:</u>

Approach temperature variables dt_{ijk}, $dt_{i,CU}$, $dt_{HU,j}$ are used to find the driving forces for Logarithmic Temperature Difference, LMTD in the area of a heat exchanger. The binary variables are utilized to invoke or suppress the presence of a match in the superstructure. If a match exists, z_{ijk} equals 1 and the constraint becomes active, which will allow the approach temperatures to be calculated properly. Conversely, if there is no match, z_{ijk} becomes zero. This will cause the contribution of the upper bound for temperature difference Γ on the right-hand side to deactivate the equality. The same is applicable to utility binary variables.

$$dt_{ijk} \leq t_{i,k} - t_{j,k} + \Gamma(1 - z_{ijk}) \qquad i \in H,\ j \in C,\ k \in K, \qquad \text{(3-16)}$$

$$dt_{ijk+1} \leq t_{i,k+1} - t_{j,k+1} + \Gamma(1 - z_{ijk}) \qquad i \in H,\ j \in C,\ k \in K, \qquad \text{(3-17)}$$

$$dt_{i,CU} \leq t_{i,NOK+1} - T_{CU}^{out} + \Gamma(1 - z_{i,CU}) \qquad i \in H, \qquad \text{(3-18)}$$

$$dt_{HU,j} \leq T_{HU}^{out} - t_{j,1} + \Gamma(1 - z_{HU,j}) \qquad j \in C, \qquad \text{(3-19)}$$

An exchanger minimum approach temperature (EMAT) is utilized to guarantee that infinite area exchangers are non-existent in the superstructure. This can be described as:

$$dt_{ijk} \geq \theta \qquad i \in H,\ j \in C,\ k \in K, \qquad \text{(3-20)}$$

where θ is a small positive value.

8. Evaluation of Relationship between stream properties:

The heat capacity as a function of stream interval and target temperatures is given as:

$$C_p = a + bT + cT^2 \tag{3-21}$$

For the interval temperature $t_{i,k}$ and $t_{j,k}$ the specific heat capacity is defined as:

$$C_{p,i,k} = a + bt_{i,k} + ct_{i,k}^2 \qquad k \in K,\ i \in H \tag{3-22}$$

$$C_{p,j,k} = a + bt_{j,k} + ct_{j,k}^2 \qquad k \in K,\ j \in C \tag{3-23}$$

$$C_{p,i}^T = a + bT_i^T + cT_i^{T\,2} \qquad i \in H \tag{3-24}$$

$$C_{p,j}^T = a + bT_j^T + cT_j^{T\,2} \qquad j \in C \tag{3-25}$$

9. Contact area for matches, *i,j*, *i,CU*, *HU,j* in stage *k*:

The required area for each match within the superstructure must be calculated according to the nature of the involved streams. The area of a match between streams is calculated by equation (3-26). On the other hand, equation (3-27) is used to determine the area for a match between a hot stream and cold utility, whereas equation (3-28) is utilized to find the area of a match involving a cold stream and hot utility.

$$A_{ijk} = \left(\frac{q_{ijk}}{\left[\left(dt_{ijk}\right)\left(dt_{ijk+1}\right)\left(\frac{dt_{ijk} + dt_{ijk+1}}{2}\right) \right]^{\frac{1}{3}}} \right) \times \left(\frac{1}{h_i} + \frac{1}{h_j} \right),\ i \in H,\ j \in C,\ k \in K \tag{3-26}$$

$$A_{i,CU} = \left(\frac{q_{i,CU}}{\left[\left(dt_{CU,i} \right) \left(T_i^T - T_{CU}^S \right) \left(\frac{dt_{i,CU} + T_i^T - T_{CU}^S}{2} \right) \right]^{\frac{1}{3}}} \right) \times \left(\frac{1}{h_i} + \frac{1}{h_j} \right), \; i \in H \qquad (3\text{-}27)$$

$$A_{HU,j} = \left(\frac{q_{HU,j}}{\left[\left(dt_{HU,j} \right) \left(T_{HU}^S - T_j^T \right) \left(\frac{dt_{HU,j} + T_{HU}^S - T_j^T}{2} \right) \right]^{\frac{1}{3}}} \right) \times \left(\frac{1}{h_i} + \frac{1}{h_j} \right), \; j \in C \qquad (3\text{-}28)$$

Note that the LMTD_{ijk} in equations (26-28) is calculated using the Chen approximation (1987).

10. <u>Objective function:</u>

The total annual cost is the objective function that must be minimized. The function includes the utility cost, exchangers fixed charges and area cost for each exchanger as follows:

$$\min \sum_{i \in H} CCUq_{i,CU} + \sum_{j \in C} CHUq_{HU,j} + \sum_{i \in H} \sum_{j \in C} \sum_{k \in K} CF_{i,j} C_{p_{i,j}} z_{ijk} + \sum_{i \in H} CF_{i,CU} C_{p_{i,CU}} z_{i,CU}$$

$$+ \sum_{j \in C} CF_{HU,j} C_{pHU,j} z_{HU,j} + \sum_{i \in H} \sum_{j \in C} \sum_{k \in K} C_{i,j} \left(A_{ijk} \right)^{\lambda_{ij}} + \sum_{i \in H} C_{i,CU} \left(A_{i,CU} \right)^{\lambda_{i,CU}}$$

$$+ \sum_{j \in C} C_{HU,j} \left(A_{HU,j} \right)^{\lambda_{HU,j}} \qquad (3\text{-}29)$$

3.5 Results and Discussion

Two case studies were developed in order to demonstrate the effectiveness of the mathematical formulation from the previous section. We were unable to use examples from literature because: (1) most examples are given in such a way that does not enable the identification of species in each stream (see table 3-1 for a sample from [7]) which is very important in identifying the appropriate heat capacity correlation; or (2) the examples involve a very high number of streams that contain mixtures of species, which is not a good idea when attempting to test a newly developed formulation. Our case studies are under the assumptions that were put forth in section 3.2.

Table 3-1: Data for an example from literature [7].

Stream	T^S (K)	T^T (K)	FC_p (kW/K)
H1	443	333	30
H2	423	303	15
C1	293	408	20
C2	353	413	40
HU	450	450	-
CU	293	313	-

With regards to the costs associated with these processes, the fixed charge for heat exchangers of any kind (process, utility) is \$5500/year. The area-dependent cost coefficient is \$300/year. Additionally, the heating utility costs \$80/kW-year while the cooling utility costs \$15/kW-year.

3.5.1 Case Study 1

The first case study is based on the reaction of ethyl acetate and sodium hydroxide to produce ethanol and sodium acetate. Table 3-2 shows the stream data for the case study. Additionally, figures 3-5 to 3-8 show the correlation between heat capacity and temperature for each species in the process. Also, the heat capacity coefficients for each stream are summarized in table 3-3.

In case study 1, the flow rate for all streams was assumed to be 200 L/min (except sodium hydroxide at 1000 L/min). The analysis is done by comparing the results of optimizing this process using the superstructure of Grossman and Yee (base Case) to results obtained from the modified superstructure derived in section 3.4. For the base case, heat capacities were assumed constant and calculated at the supply temperature. The formulation was applied on this case study for a minimum approach temperature (ΔT_{min}) of 10 K, λ equal to 1 and a two stage superstructure.

Table 3-2: Stream Data for Case Study 1.

Stream	***Compound***	***T^S (K)***	***T^T (K)***	***F (kg/s)***
H1	Water	368	318	3.33
H2	Sodium Acetate	353	313	5.10
C1	Ethyl Acetate	293	363	2.99
C2	Sodium Hydroxide	298	398	4.17
HU	Steam	680	680	-
CU	Cooling Water	300	320	-

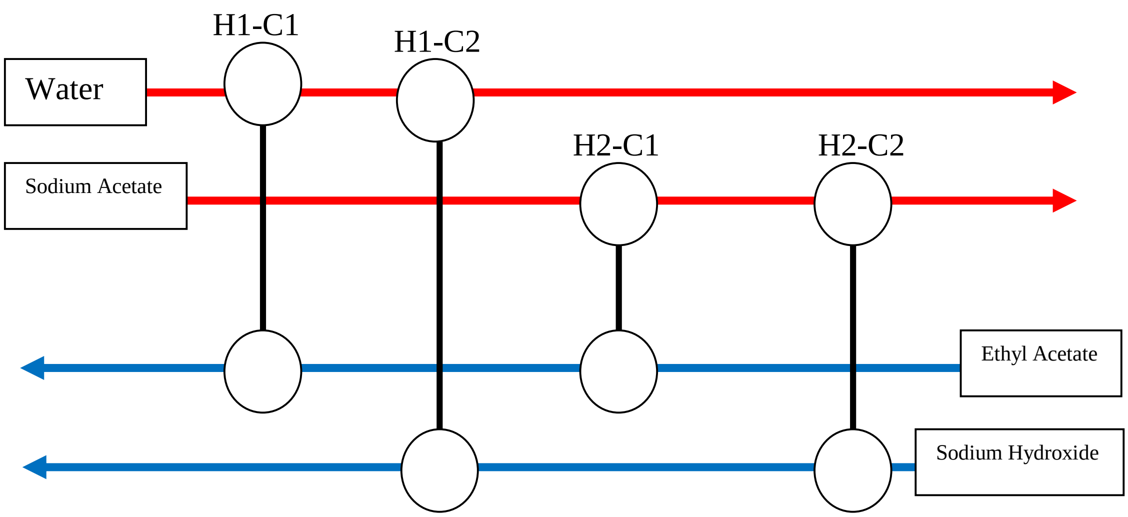

Figure 3-4: Case study 1 diagram with potential stream matches.

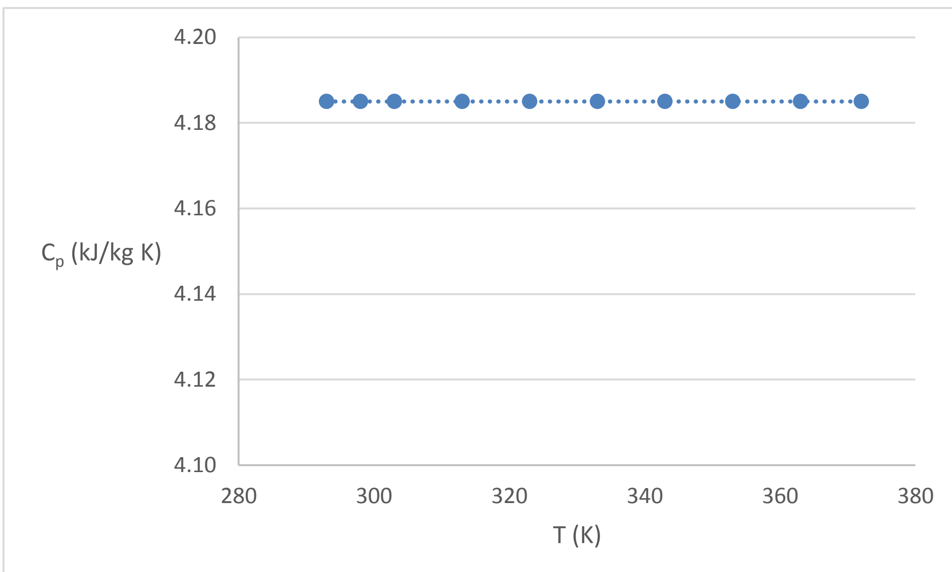

Figure 3-5: Heat capacity profile for water

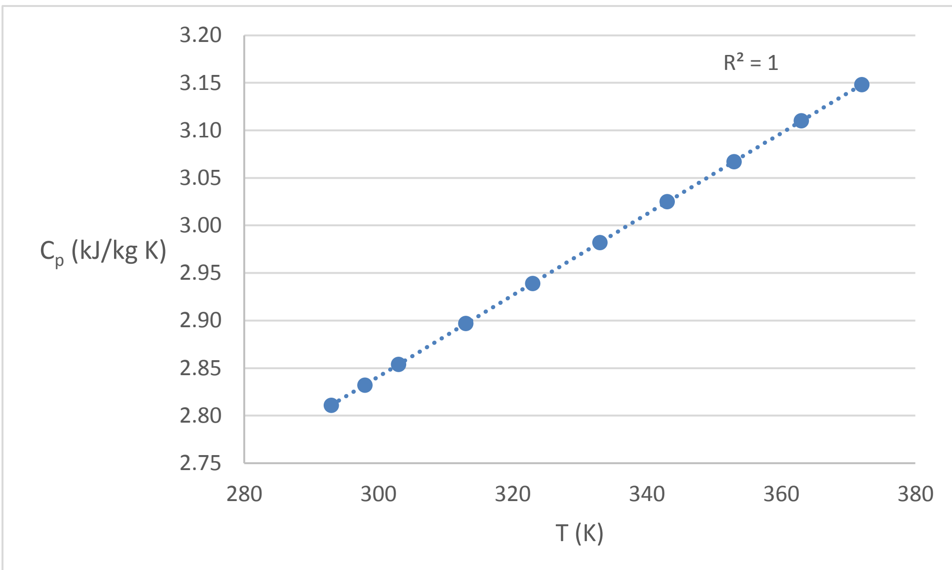

Figure 3-6: Heat capacity profile for sodium acetate.

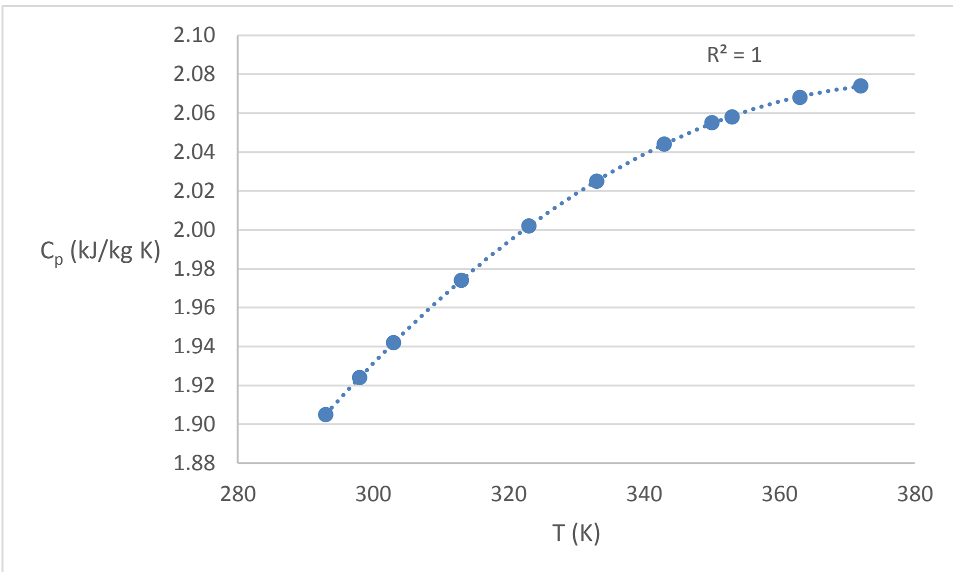

Figure 3-7: Heat capacity profile of ethyl acetate.

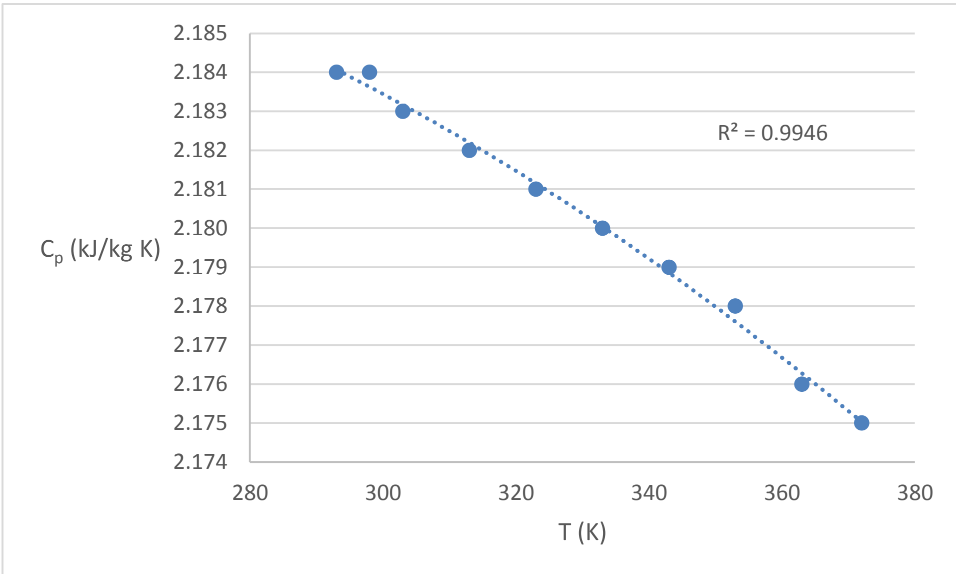

Figure 3-8: Heat capacity profile of sodium hydroxide.

Table 3-3: Heat capacity coefficients for case study 1

Species	Water	Sodium Acetate	Ethyl acetate	NaOH
a	4.185	1.56	-1.142	2.209
b	0	4.27E-03	1.69E-02	-6.24E-05
c	0	0	-2.22E-05	-7.53E-08

The results of optimization for the base case and the modified case (variable C_p) will be summarized in the next few tables and figures. They include heating loads, process exchanger areas and utility exchanger areas for all stream matches in the superstructure for both cases (see tables 3-4 and 3-5, respectively). Additionally, the temperature at each stage for all streams will be provided in table 3-6. Finally, a cost comparison is provided in table 3-7 and figure 3-9.

In our research, a mathematical formulation was introduced as the framework to solve the proposed problem. The formulation was applied to the case study shown in table 3-2. The cost comparison between the two approaches will shed light on the impact variable heat capacity can have on HEN.

Table 3-4: Results for base case 1.

Match (i,j,k)	***1,2,2***	***2,2,2***	***CU,1***	***CU,2***	***HU,1***	***HU,2***
q (kW)	530.1	359.72	167.4	265.9	399.0	3659.2
Area (m^2)	4.13	2.94	13.8	25.2	0.405	4.5

Table 3-5: Results for modified formulations (case 1).

Match (i,j,k)	***1,2,2***	***2,2,2***	***CU,1***	***CU,2***	***HU,1***	***HU,2***
q (kW)	529.6	525.1	167.2	373.3	576.0	3398.9
Area (m^2)	4.32	4.55	13.8	35.3	0.584	4.20

Table 3-6: Stage interval temperatures (K) (case 1).

Base Case	***k=1***	***k=2***	***k=3***	***Var. Cp.***	***k=1***	***k=2***	***k=3***
H1	368	368	330	**H1**	368	368	330
H2	353	353	330	**H2**	353	353	330
C1	293	293	293	**C1**	293	293	293
C2	317.6	317.6	298	**C2**	321.6	321.6	298

Table 3-7: Cost comparison for case study 1.

Base Case	***Cost ($/yr)***	***Var. C_p.***	***Cost ($/yr)***
Heating utility	324654	**Heating utility**	317991
Cooling utility	6499	**Cooling utility**	8108
Fixed costs	40640	**Fixed costs**	42415
TAC	371794	**TAC**	368514

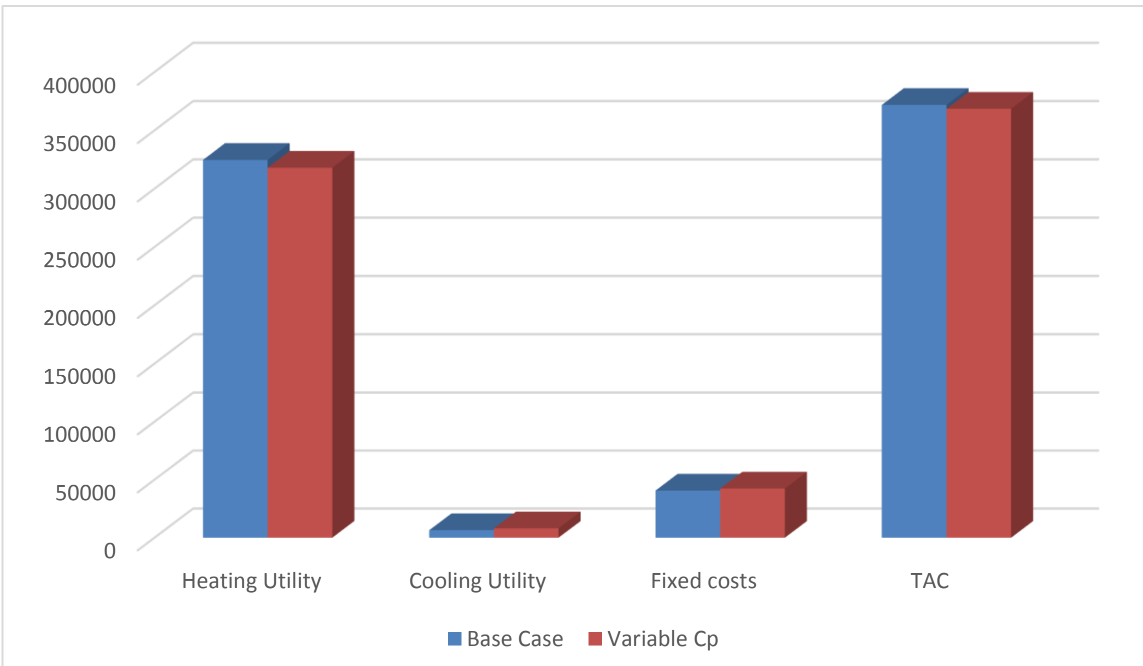

Figure 3-9: Costs comparison for case study 1.

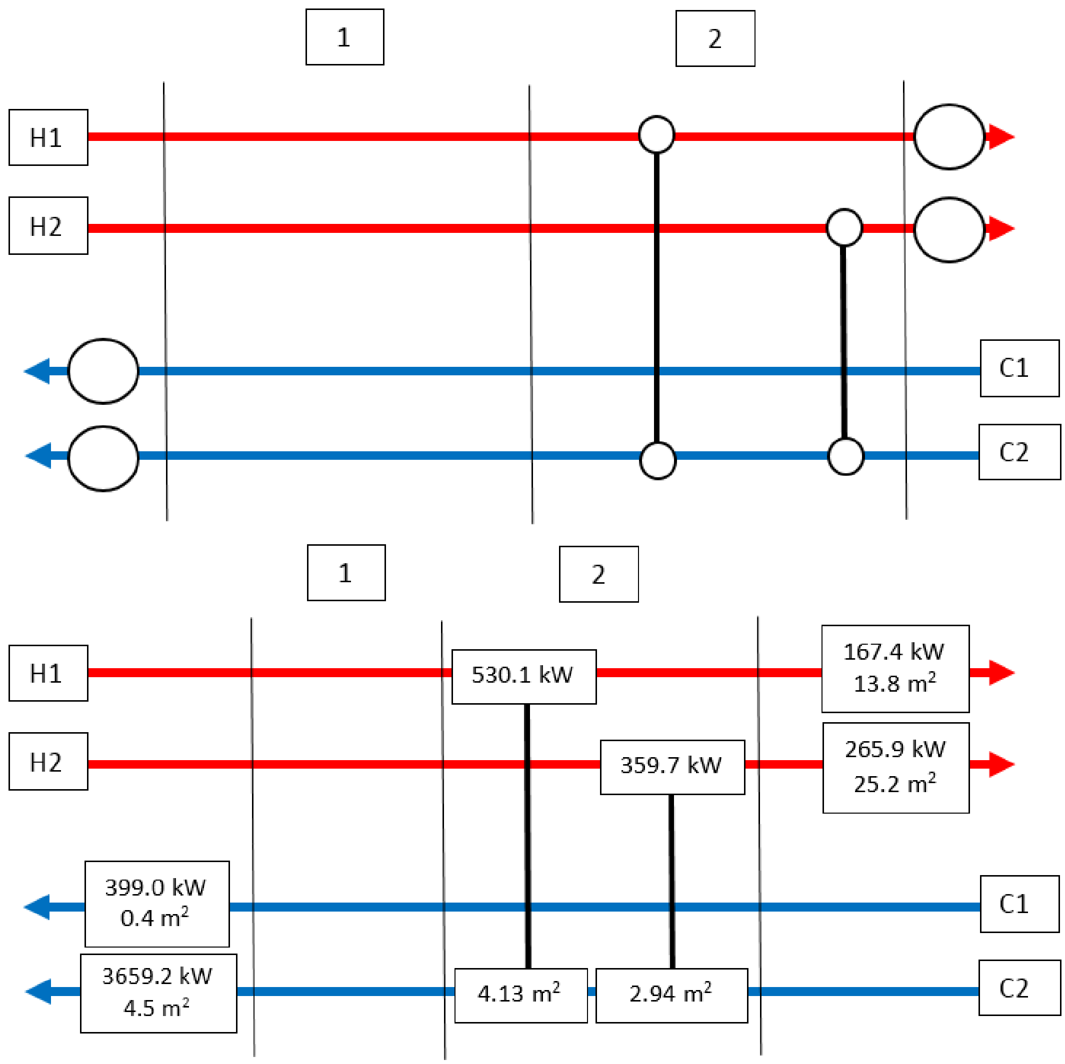

Figure 3-10: Graphical summary of base case 1

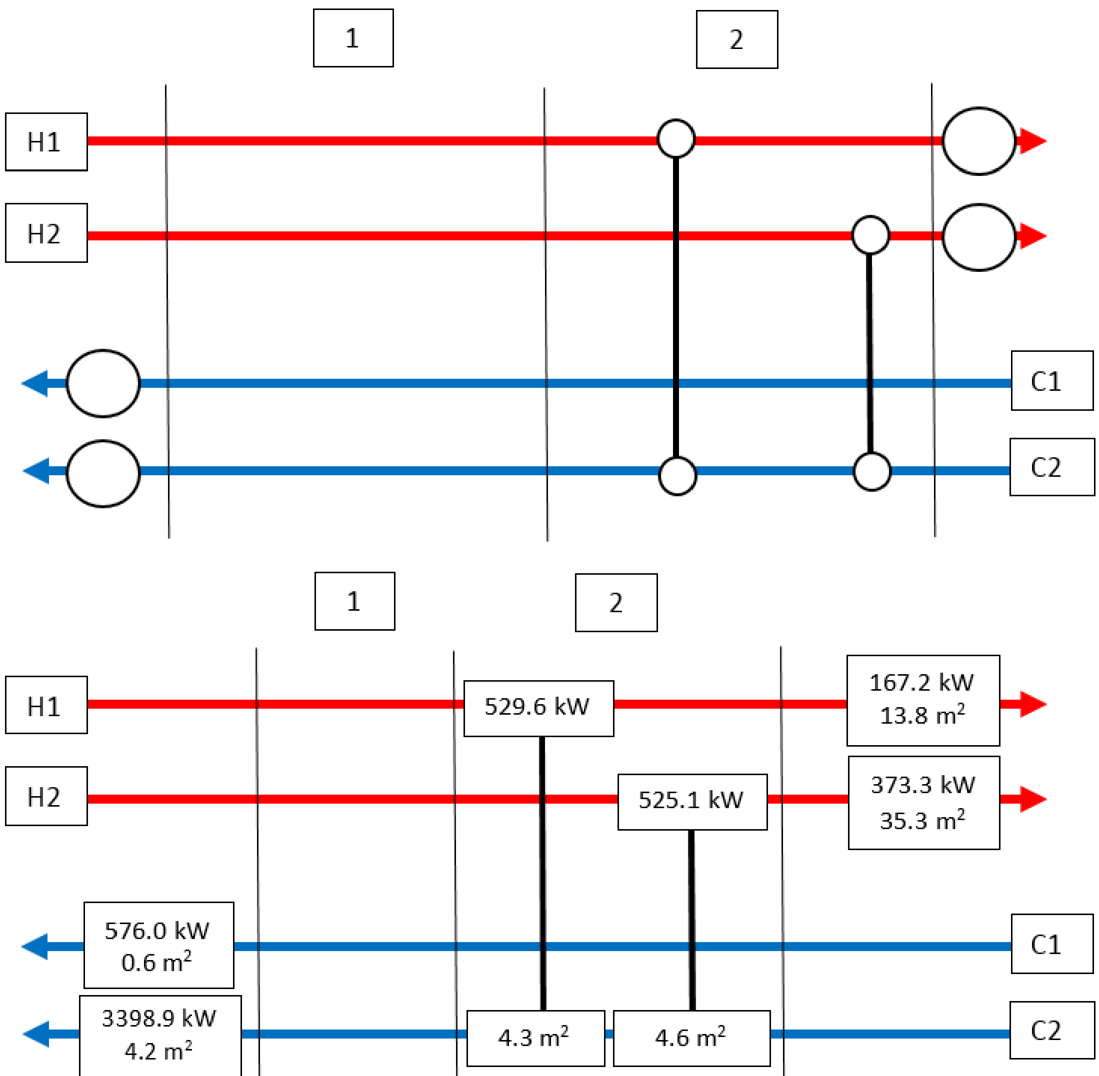

Figure 3-11: Graphical summary of variable Cp case 1

Table 3-7 shows the costs associated with both HENs. Overall, the costs have somewhat changed when variable heat capacity was considered. Hot and cold utilities have changed by -2.1% and 24.8%, respectively. By considering these changes with a fixed cost increase of 4.4%, the total annual cost (TAC) has become 0.9% lower than TAC for the base case, evidenced by observing figure 3-9.

A look at the different utility loads between the two cases can be beneficial in understanding these variable costs. According to tables 3-4 and 3-5, the total utility heating load has decreased from 4058.2 kW in the base case to 3974.9 kW and total utility cooling load has increased from 433.3 to 540.5 kW. These results correspond to -2.1% and 24.7% changes in utility heating and cooling loads, respectively.

The variable heat capacity has given rise to a higher energy requirement for either heating or cooling as we go from right to left in the superstructure and thus, a slightly modified amount of utility must be used which resulted in a small decrease of TAC by around 1%.

Table 3-6 shows that C1 did not get involved in the process-to-process (PTP) heat exchange. H1 and H2 preferred matching with C2 due to its higher heat content resulting from its relatively higher heat capacity and flow rate. Because of this, the optimum HEN exhibits a much higher heating utility cost to accommodate the heating targets for C1 and C2. A summary in the form of a grid diagram is presented in figures 3-10 and 3-11.

3.5.2 Case Study 2

The second case study is based on the reaction of benzene and ethylene to produce ethyl benzene and the further reformation of ethyl benzene to produce styrene. Table 3-8 shows the stream data for the case study. Additionally, figures 3-13 to 3-15 show the correlation between heat capacity and temperature for each species in the process. Also, the heat capacity coefficients for each stream are summarized in table 3-9.

In case study 2, the flow rate for all streams was also assumed to be 200 L/min. The same analysis plan discussed in section 3.5.1 is to be followed. Similarly for the base case, heat capacities were assumed constant and calculated at the supply temperature. The formulation was applied on this case study for a minimum approach temperature (ΔT_{min}) of 10 K, λ equal to 1 and a two stage superstructure as well.

Table 3-8: Stream data for case study 2

Stream	Compound	T^S (K)	T^T (K)	F (kg/s)
H1	Ethyl benzene	358	313	2.89
H2	Styrene	348	308	3.03
C1	Benzene	303	348	2.92
C2	Water	308	323	3.33
HU	Steam	680	680	-
CU	Cooling Water	300	320	-

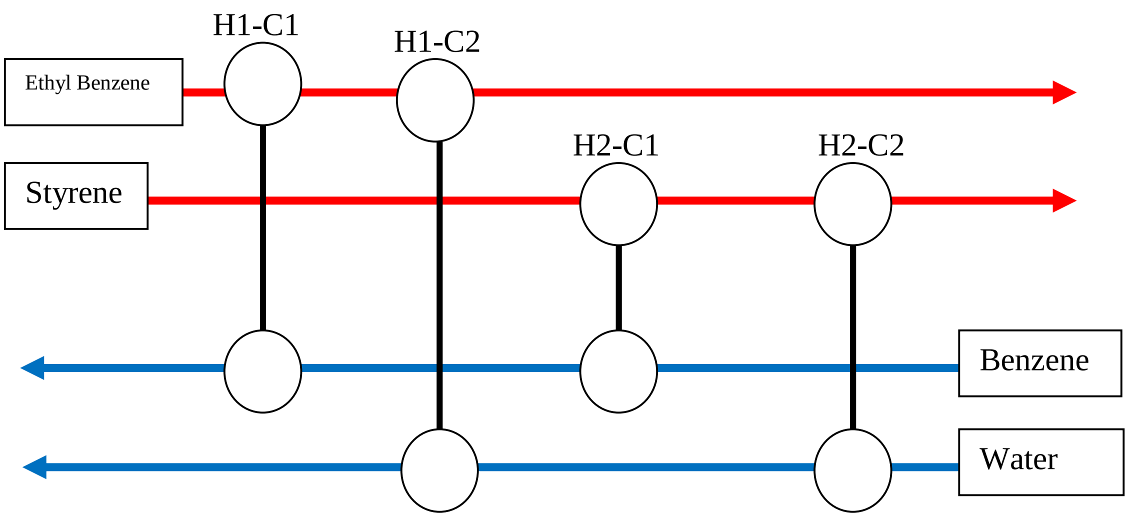

Figure 3-12: Case study 2 diagram with potential stream matches.

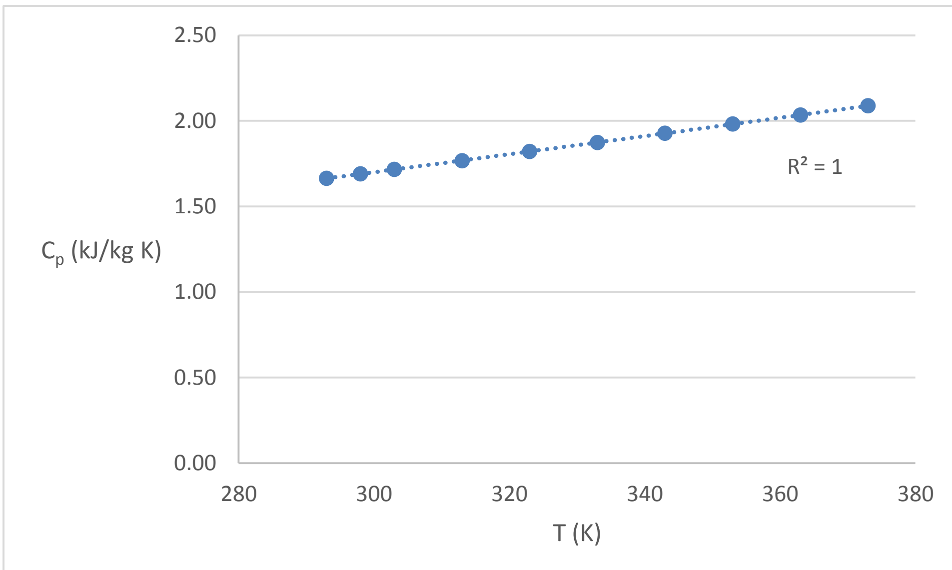

Figure 3-13: Heat capacity profile of ethyl benzene.

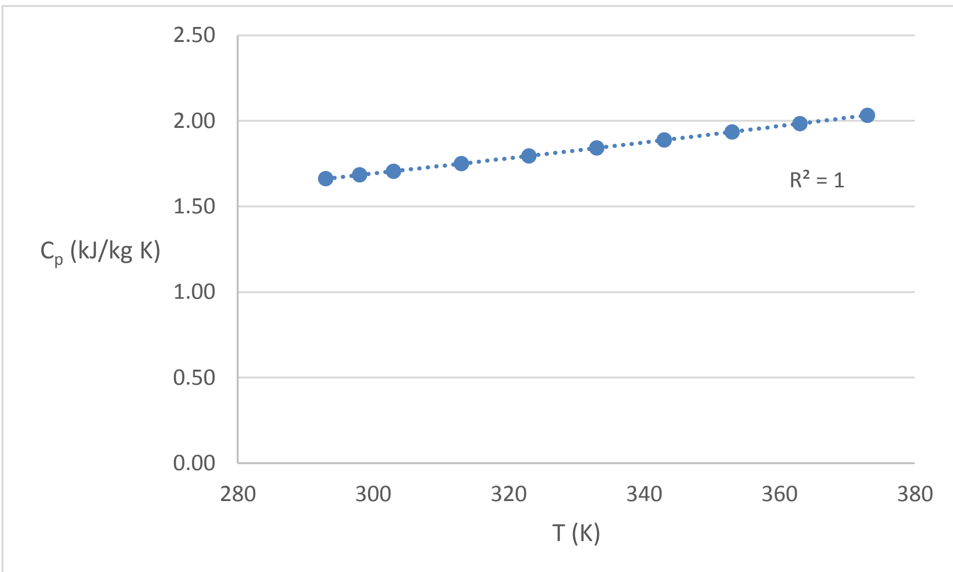

Figure 3-14: Heat capacity profile for styrene.

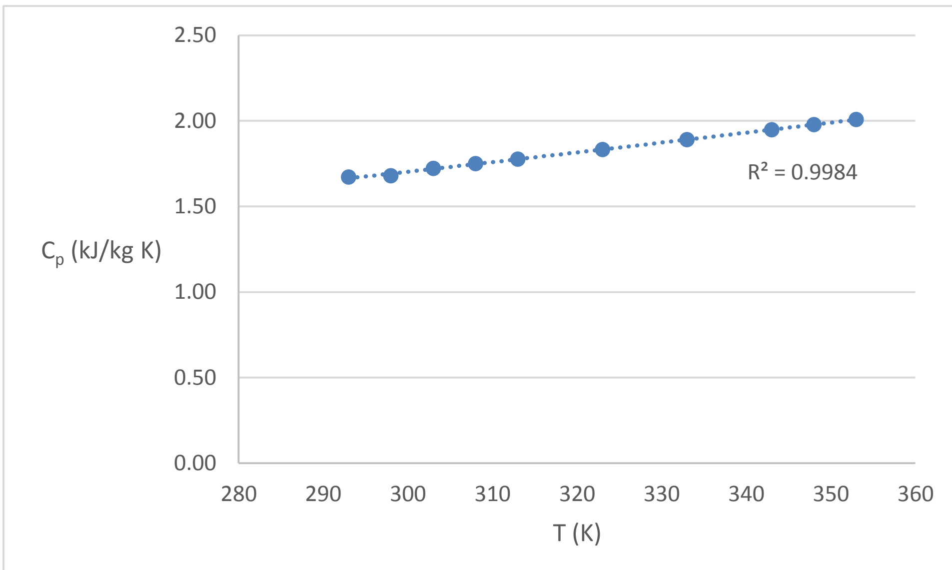

Figure 3-15: Heat capacity profile for benzene

Table 3-9: Heat capacity coefficients for case study 2.

Species	Ethyl Benzene	Styrene	Benzene	Water
a	2.59E-01	7.40E-01	3.43E-01	4.185
b	4.39E-03	1.97E-03	3.50E-03	0
c	1.37E-06	4.01E-06	3.44E-06	0

The same mathematical formulation was applied on the second case study and results were collected for both the base case and the variable heat capacity case. Heating loads, process exchanger areas and utility exchanger areas are summarized in tables 3-10 and 3-11, respectively. Also, the interval temperatures at each stage are provided in table 3-12. Finally, table 3-13 and figure 3-16 illustrate the cost comparisons for each case. A graphical summary of the results can be seen in figures 3-17 and 3-18.

From table 3-13, it can be observed that costs have changed slightly with the exception of cooling utility, which increased by 45.6% compared to the base case. Heating utility has decreased by 2.3% and fixed costs have risen by 4.5%. Taken as a whole, all costs associated with the process ultimately caused the TAC to increase by 5.1%. These trends can be seen by looking at figure 3-16 as well.

According to tables 3-10 and 3-11, hot utility has declined slightly between the two formulations. However, cold utility has risen from 266.2 to 387.1 kW, which corresponds to a 45.4% increase that is reflected on the cold utility cost. These changes in costs can be attributed to the increase in heat capacity from right to left in the superstructure.

Comparing the fixed costs for case studies 1 and 2 shows that variability in heat capacity has minimal impact compared to its effects on utility costs. By looking at the formulation in section 3.4, we can see that heat capacity is directly involved in the energy balances that dictate utility loads, whereas the heat exchanger design equations do not involve heat capacity. Thus, its effect on fixed costs is minimized.

Table 3-10: Results for base case 2.

Match (i,j,k)	1,1,1	2,1,2	CU,1	CU,2	HU,2
q (kW)	157.8	68.5	103.2	163.1	209.3
Area (m^2)	11.1	1.80	14.4	23.1	0.145

Table 3-11: Results for modified formulation (case 2)

Match (i,j,k)	**1,1,1**	**1,2,1**	**2,1,1**	**CU,1**	**CU,2**	**HU,1**
q (kW)	95.6	209.2	188.7	172.3	214.8	204.5
Area (m^2)	2.90	5.32	7.03	25.0	39.3	0.230

Table 3-12: Stage interval temperatures (K) (case 2).

Base Case	**k=1**	**k=2**	***k*=3**	**Var. C_p**	**k=1**	**k=2**	***k*=3**
H1	358	330.8	330.8	**H1**	358	330	330
H2	348	348	336.2	**H2**	348	330	330
C1	348	316.6	303	**C1**	330.1	303	303
C2	308	308	308	**C2**	323	308	308

Table 3-13: Costs comparison for case study 2.

Base Case	Cost ($/yr)	Var. C_p	Cost ($/yr)
Heating utility	16740	**Heating utility**	16363
Cooling utility	3994	**Cooling utility**	5807
Fixed costs	62578	**Fixed costs**	65368
TAC	83312	**TAC**	87538

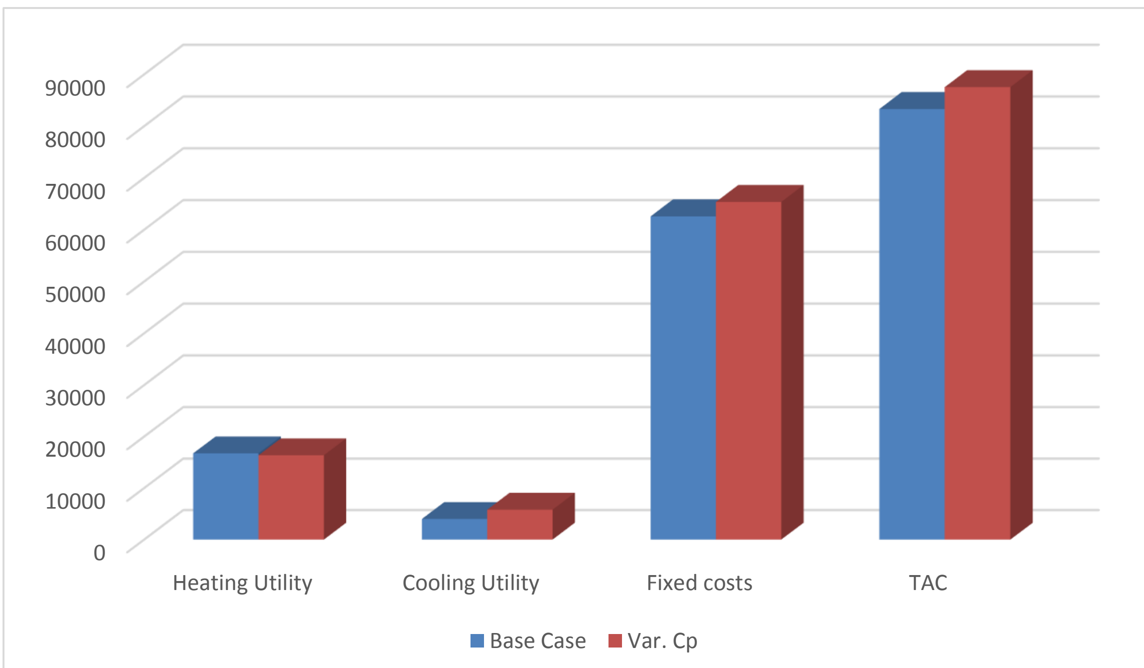

Figure 3-16: Costs comparison for case study 2.

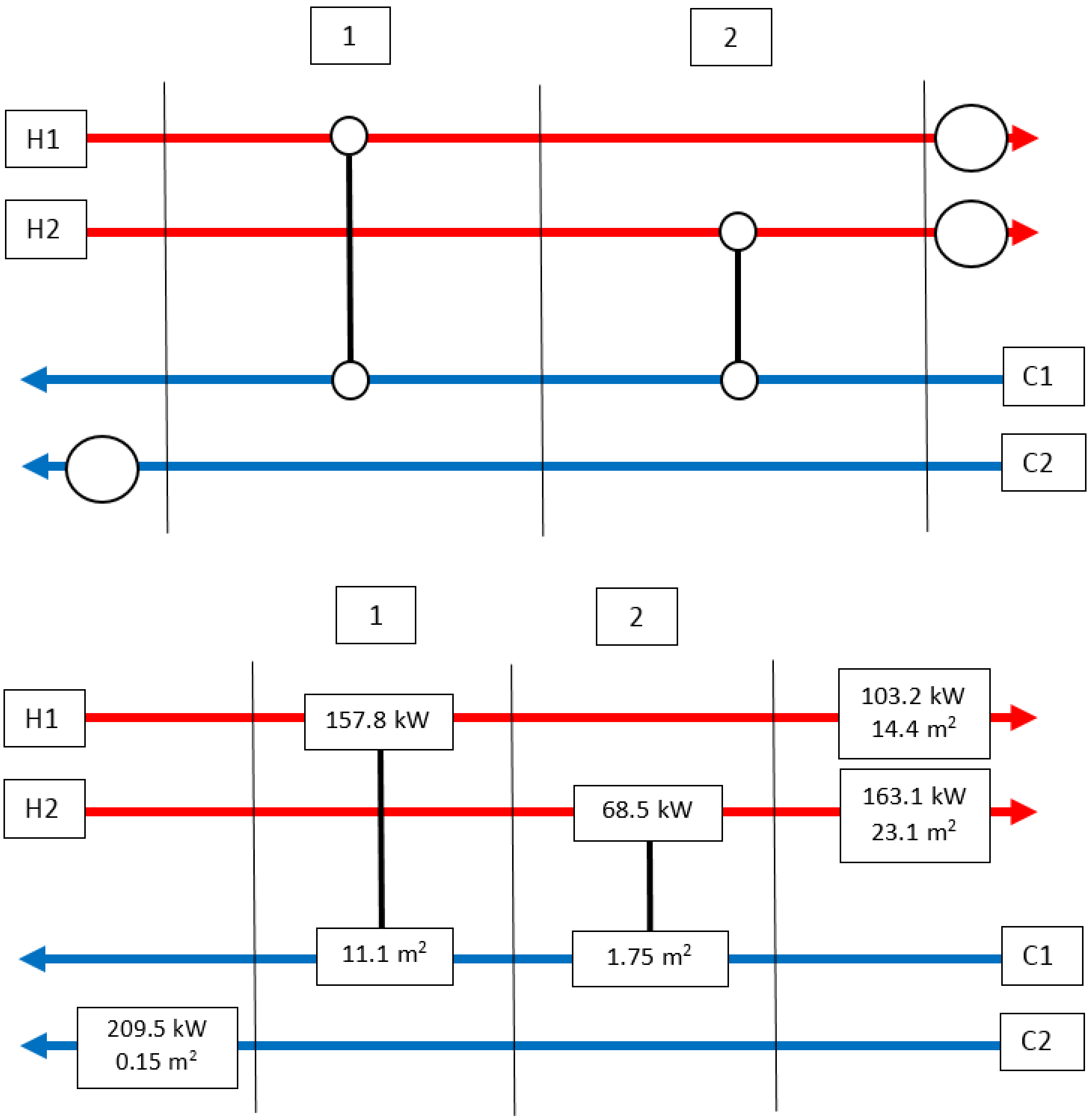

Figure 3-17: Graphical summary of base case 2

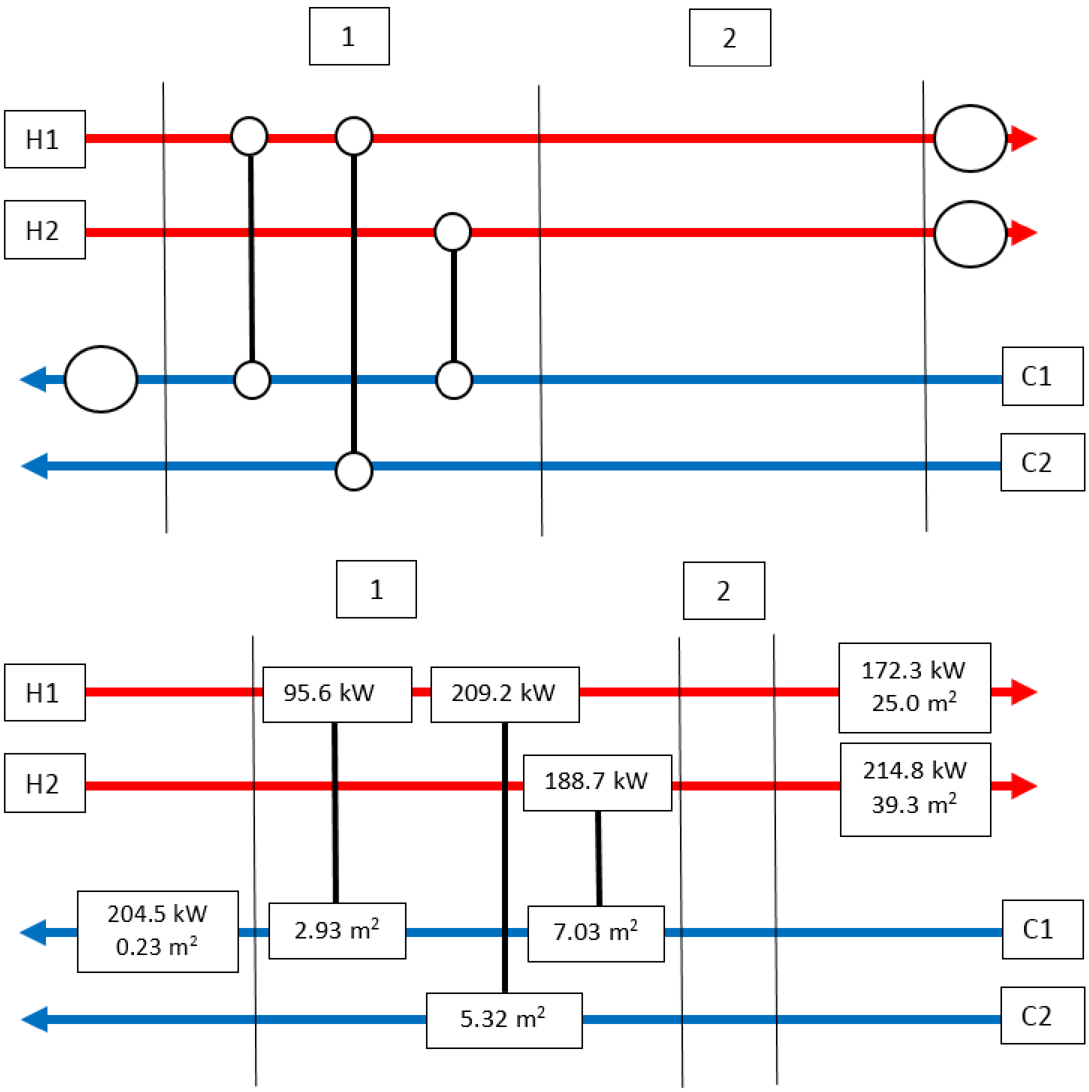

Figure 3-18: Graphical summary of variable Cp case 2.

CHAPTER 4

EFFECTS OF STREAM PROPERTY PROFILES ON THE OPTIMIZATION OF HEAT EXCHANGER NETWORKS

In this chapter, stream properties other than heat capacity will be introduced to the mathematical formulation in order to investigate their impact on the optimum HEN. First, we start by covering variability of viscosity, thermal conductivity and heat transfer coefficient with temperature. Then, we present the methodology to tackle the problem of optimum HEN under variable stream properties. Next, the mathematical formulation will be developed. Finally, the chapter concludes with results from applying the formulation to the same case studies from chapter 3 and a discussion of those results will be provided.

4.1 Background

In chapter 3, heat capacity was considered a variable function of temperature. This modification to the formulation has created a change in optimum HENs for two different case studies. In order to further investigate the effects of variability, we will modify the formulation even more to account for variability in other stream properties. In particular, we will focus on viscosity, thermal conductivity and heat transfer coefficient (h).

Viscosity can be defined as the measurement of the internal fluid friction under a shearing stress. In reality, viscosity tends to vary with temperature and pressure for different species. Its effect on the superstructure will mostly be seen in the equations of heat exchanger design rather than the energy balances.

In literature, most process optimization examples (see table 3-1) assume a constant heat transfer coefficient. This implies that the viscosity is also constant. By introducing heat transfer parameters such as Reynolds (*Re*), Prandtl (*Pr*) and Nusselt (*Nu*) numbers to the formulation, we can control variability by replacing constant viscosity, thermal conductivity and heat transfer coefficient with their corresponding variable correlations.

Viscosity varies greatly with temperature. However, its relationship with pressure is more complex depending on the phase of the system under investigation. Figure 4-1 shows how the viscosity of carbon dioxide is effected by pressure and temperature. We can see that for species in the gas phase, the pressure can have as much impact as temperature on viscosity. On the other hand, if we look at figure 4-2 showing the effects of pressure on viscosity of liquids, we observe very minimal effect on reduced viscosity when the reduced pressure (P_r) is sufficiently low (i.e. $0 < P_r < 2$). Thus, it can be said that:

$$\mu = \mu(T) \qquad \text{(low pressure, liquid phase)} \qquad (4\text{-}1)$$

There are some correlations in literature that involve the prediction of viscosity for any temperature given a species, independent of pressure. One such equation takes the following form [35]:

$$\ln \mu = a + b \ln T \qquad (4\text{-}2)$$

The constants a and b in equation (4-2) are coefficients that differ for each species. Table 4-1 shows their values for some compounds.

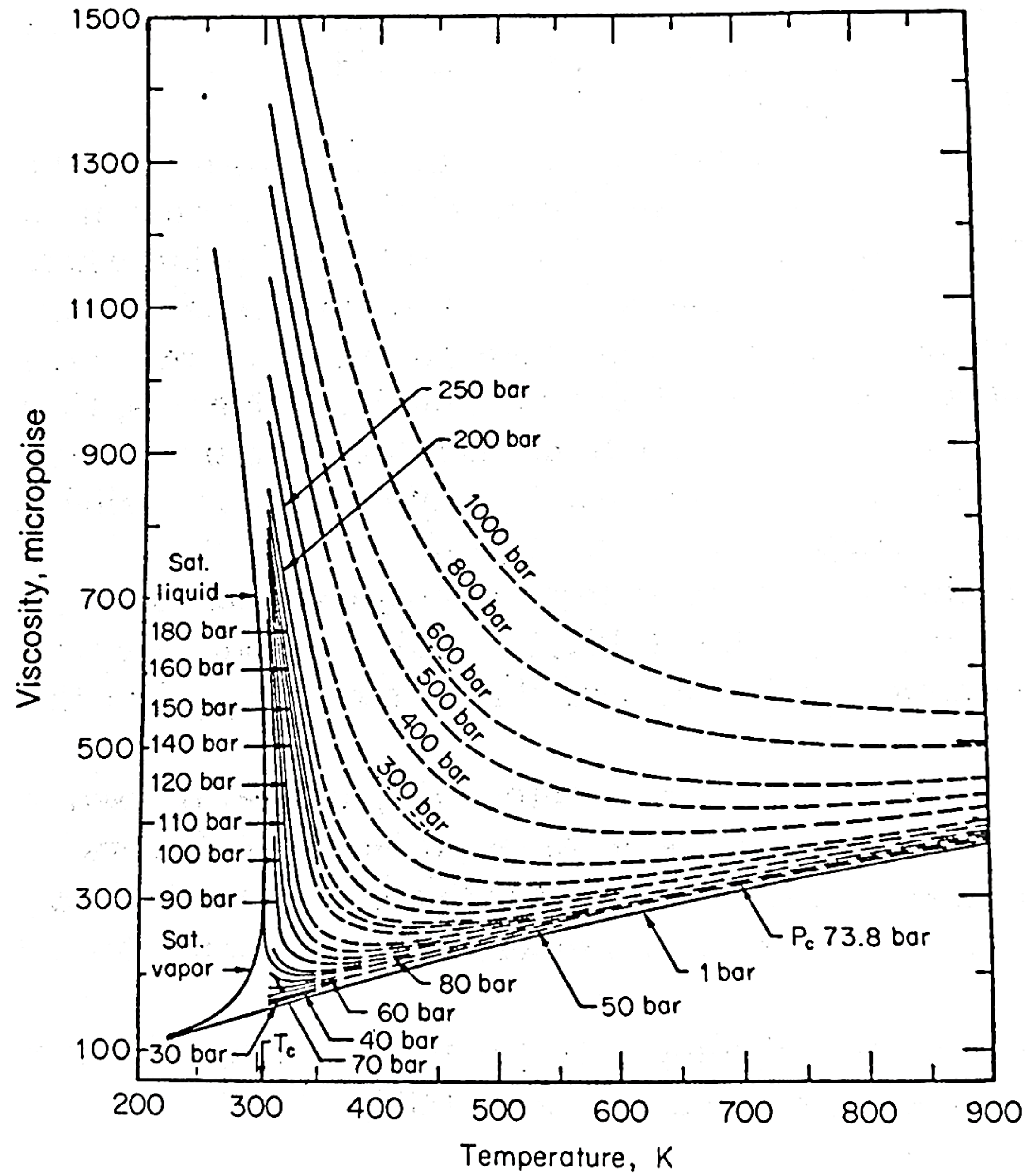

Figure 4-1: Viscosity of carbon dioxide, gas phase [34].

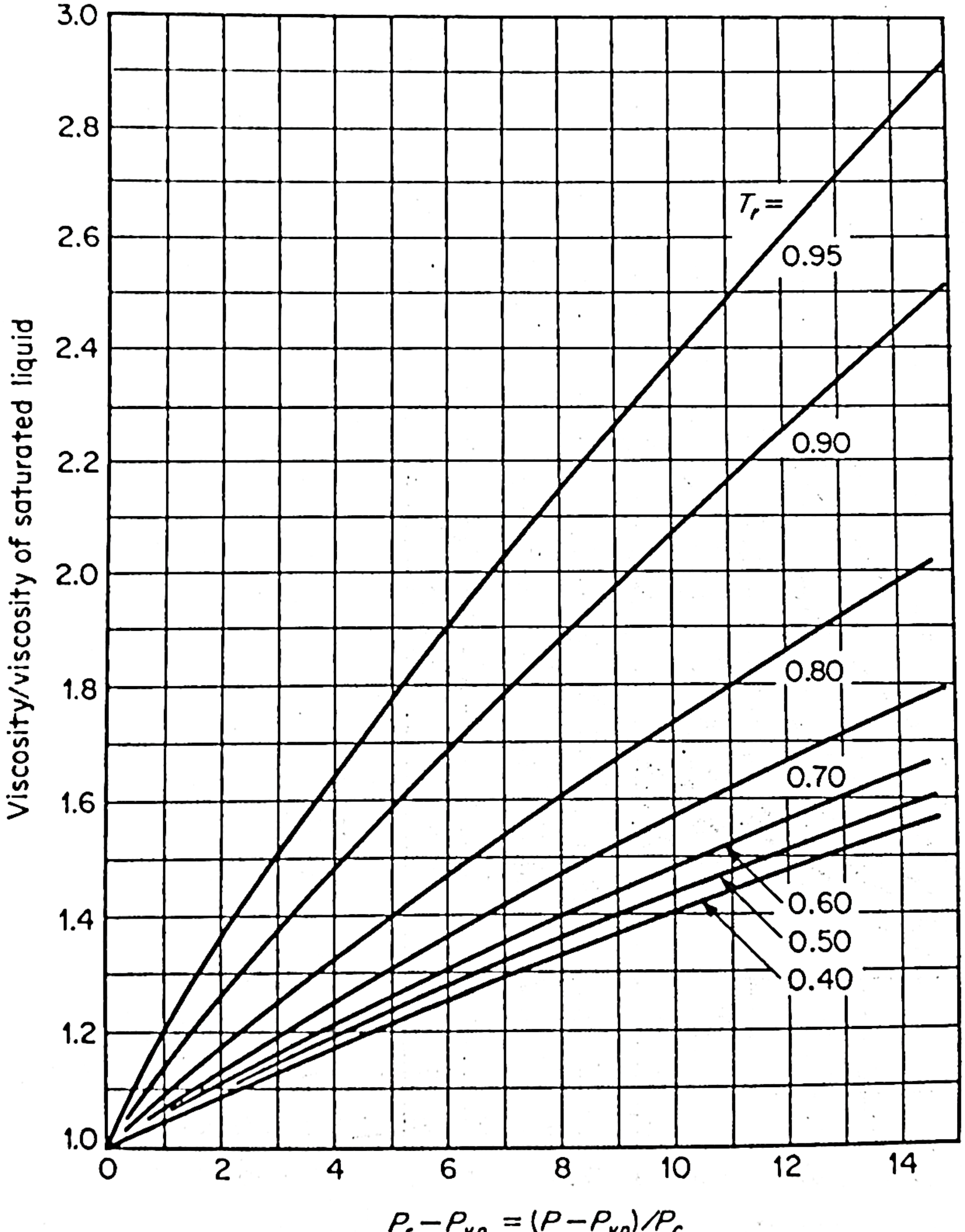

Figure 4-2: Effect of pressure on viscosity of liquids [34].

Table 4-1: Viscosity coefficients for liquids [35].

Liquids	a (T in K)	b (T in K)
Acetone	14.64	-2.77
Benzene	21.99	-3.95
Crude Oil, 35^{o} API	53.73	-9.01
Ethanol	31.63	-5.53
Glycerol	106.76	-17.60
Kerosene	33.41	-5.72
Methanol	22.18	-3.99
Octane	17.86	-3.25
Pentane	13.46	-2.62
Water	29.76	-5.24

For the purposes of this research, viscosity and thermal conductivity data versus temperature will be collected from ASPEN HYSYS. These variables will be used in tandem with other properties such as heat capacity and density as part of the design of heat exchangers in the superstructure. By calculating *Re*, *Pr* and *Nu* for each species for a certain temperature range, we can calculate the heat transfer coefficient h for various temperatures. This will be useful in creating a curve fit for h versus T corresponding to a species and thus, we can introduce it to the formulation to investigate the effects of stream property profiles on optimum HEN. The curve fit for h will be a polynomial of order 2 as follows:

$$h = \alpha + \beta T + \gamma T^2 \tag{4-3}$$

These issues and more will be discussed thoroughly in the methodology and mathematical formulation sections of this chapter.

4.2 Methodology

The plan in this part of the research is to follow a path similar to section 3.2 from the previous chapter. A MINLP model will be formulated that takes into consideration the stream property profiles. *Hence, we will develop models that account for changes in physical properties such as heat capacities, viscosities, thermal conductivities and heat transfer coefficients.* We will again use the formulation of Grossman and Yee (1990) as a basis for our modifications. The following is a reminder of the assumptions to be made in the mathematical formulation:

(1) There will only be one type of hot utility and cold utility (i.e. steam and water).

(2) Hot and cold utilities will be placed outside the superstructure the represents the HEN.

(3) The process involves isothermal-mixing only.

(4) Each stream contains pure, incompressible fluid species in the liquid phase.

(5) The heat exchangers in the superstructure have a double-pipe configuration.

In light of this chapter, some of the assumptions above have a significant impact on our new formulation. The 4th assumption implies that the density of each species in the superstructure is constant. Forcing the streams to be in liquid phase will eliminate pressure effects on the viscous forces (i.e. viscosity) while having a more significant role in changing the flow regime (i.e. *Re*) due to pressure's more present impact on the inertial forces.

On the other hand, the 5th assumption is useful in choosing an appropriate correlation to calculate the heat exchanger design parameters. In this research, cold streams will flow in the inner pipe (1-inch, Schedule 40), whereas hot streams will flow in the outer pipe (2-inch, Schedule 40). Figure 3-1 clarifies this configuration.

The software packages discussed in section 3.2 will be used in this case as well. DICOPT will be used as a solver from the optimizing program GAMS, while thermodynamic properties will be sourced from ASPEN HYSYS unless otherwise stated.

4.3 Problem Statement

The Heat Exchanger Network Synthesis (HENS) problem can now be modified to include the goals of this chapter as follows:

"Given a number of hot process stream, N_H, that needed to be cooled and a number, N_U, of cold process stream that needed to be heated. Supply temperature, Ts, and target temperature T_T, of each stream are also provided. Available for use are heating and cooling utilities, Q_{HU}, and Q_{CU}, respectively, whose costs, supply temperatures, and target temperatures are given. Also given are the stream mass flow rate (F) or volumetric flow rate (Q). The stream heat capacity C_p is defined as a function of stream interval and target temperatures. Also defined is the stream heat transfer coefficient (h) as a function of heat exchanger geometry, stream properties embedded in the Nusselt number and thermal conductivity. It is desired to synthesize an optimal and cost effective heat exchanger networks which can transfer heat from hot process streams and hot utilities to cold process stream and cold utilities for varying process stream properties."

The objective then is to design a heat exchanger network which exhibits minimum TAC and optimum performance when subjected to stream property profiles. The basis of the formulation is identical to chapter 3 (2 hot, 2 cold streams) and figures 3-2 and 3-3 show a graphical representation of the superstructure.

4.4 Mathematical Formulation

The formulation will follow the same format set forth in section 3.4. However, new equations will be introduced to allow for more variable stream properties and heat exchanger design considerations.

Constraints

1. Overall energy balance for each stream:

$$\left(T_i^S C_{p,i}^S - T_i^T C_{p,i}^T\right)F_i = \sum_{k\in K}\sum_{j\in C} q_{ijk} + q_{i,CU} \qquad i \in H \tag{4-4}$$

$$\left(T_j^T C_{p,j}^T - T_j^S C_{p,j}^S\right)F_j = \sum_{k\in K}\sum_{i\in H} q_{ijk} + q_{HU,j} \qquad j \in C \tag{4-5}$$

2. Heat balance at each interval:

$$\left(t_{i,k} C_{p,i,k} - t_{i,k+1} C_{p,i,k+1}\right)F_i = \sum_{j\in C} q_{ijk} \qquad k \in K,\ i \in H \tag{4-6}$$

$$\left(t_{j,k} C_{p,j,k} - t_{j,k+1} C_{p,j,k+1}\right)F_j = \sum_{i\in C} q_{ijk} \qquad k \in K,\ j \in C \tag{4-7}$$

3. Assignment of superstructure inlet temperatures:

$$T_i^S = t_{i,1}, \qquad i \in H \tag{4-8}$$

$$T_j^S = t_{j,NOK+1,} \qquad j \in C \tag{4-9}$$

4. Temperatures feasibility:

$$t_{i,k} \ge t_{i,k+1} \qquad k \in K,\ i \in H \tag{4-10}$$

$$t_{j,k} \ge t_{j,k+1} \qquad k \in K,\ j \in C \tag{4-11}$$

$$T_i^T \le t_{i,NOK+1} \qquad i \in H \qquad (4\text{-}12)$$

$$T_j^T \ge t_{j,1} \qquad j \in C \qquad (4\text{-}13)$$

5. Energy balance for the hot and cold utility loads:

$$\left(t_{i,NOK+1} C_{p,i,NOK+1} - T_i^T C_{p,i}^T\right) F_i = q_{i,CU} \qquad i \in H \qquad (4\text{-}14)$$

$$\left(T_j^T C_{p,j}^T - t_{j,1} C_{p,j,1}\right) F_j = q_{HU,j} \qquad j \in C \qquad (4\text{-}15)$$

6. Logical constraints:

$$q_{ijk} - \Omega z_{ijk} \le 0, \qquad i \in H,\ j \in C,\ k \in K, \qquad (4\text{-}16)$$

$$q_{i,CU} - \Omega z_{i,CU} \le 0, \qquad i \in H, \qquad (4\text{-}17)$$

$$q_{HU,j} - \Omega z_{HU,j} \le 0, \qquad j \in C, \qquad (4\text{-}18)$$

$$z_{ijk},\ z_{i,CU},\ z_{HU,j} = 0,1$$

7. Heat exchanger area calculation:

$$dt_{ijk} \le t_{i,k} - t_{j,k} + \Gamma\left(1 - z_{ijk}\right) \qquad i \in H,\ j \in C,\ k \in K, \qquad (4\text{-}19)$$

$$dt_{ijk+1} \le t_{i,k+1} - t_{j,k+1} + \Gamma\left(1 - z_{ijk}\right) \qquad i \in H,\ j \in C,\ k \in K, \qquad (4\text{-}20)$$

$$dt_{i,CU} \le t_{i,NOK+1} - T_{CU}^{out} + \Gamma\left(1 - z_{i,CU}\right) \qquad i \in H, \qquad (4\text{-}21)$$

$$dt_{HU,j} \le T_{HU}^{out} - t_{j,1} + \Gamma\left(1 - z_{HU,j}\right) \qquad j \in C, \qquad (4\text{-}22)$$

$$dt_{ijk} \geq \theta \qquad i \in H\ , j \in C\ , k \in K, \qquad (4\text{-}23)$$

where θ is a small positive value.

8. Evaluation of Relationship between stream properties:

$$C_p = a + bT + cT^2 \qquad (4\text{-}24)$$

For the interval temperature $t_{i,k}$ and $t_{j,k}$ the specific heat capacity is defined as:

$$C_{p,i,k} = a + bt_{i,k} + ct_{i,k}^2 \qquad k \in K\ ,\ i \in H \qquad (4\text{-}25)$$

$$C_{p,j,k} = a + bt_{j,k} + ct_{j,k}^2 \qquad k \in K\ ,\ j \in C \qquad (4\text{-}26)$$

$$C_{p,i}^T = a + bT_i^T + cT_i^{T\,2} \qquad i \in H \qquad (4\text{-}27)$$

$$C_{p,j}^T = a + bT_j^T + cT_j^{T\,2} \qquad j \in C \qquad (4\text{-}28)$$

The viscosity as a function of stream temperatures is given as:

$$\mu = \mu(T) \qquad (4\text{-}1)$$

The thermal conductivity as a function of stream temperatures is given by:

$$\zeta = \zeta(T) \qquad (4\text{-}29)$$

For fluids at high or moderate Reynolds number (3000 < Re < 5×10^6) in double-pipe heat exchangers, the Nusselt number can be estimated using the following correlations [32]:

$$N_{u,i} = 0.023(\mathrm{Re}_i)^{0.8}(\mathrm{Pr}_i)^{0.3} \qquad i \in H \qquad (4\text{-}30)$$

The Reynolds number is defined as:

$$\mathrm{Re}_i = \frac{4\rho_i Q_i}{\pi\mu_i D} \qquad i \in H \qquad (4\text{-}31)$$

The Prandtl number is defined as:

$$\mathrm{Pr}_i = \frac{C_{p,i}\mu_i}{\zeta_i} \qquad i \in H \qquad (4\text{-}32)$$

Then, heat transfer coefficient can be calculated as:

$$h_i = \frac{N_{u,i}\zeta_i}{D_i} \qquad i \in H \qquad (4\text{-}33)$$

For cold streams, the same correlation can be used with a small modification to Nusselt number calculation [32]:

$$N_{u,j} = 0.023(\mathrm{Re}_j)^{0.8}(\mathrm{Pr}_j)^{0.4} \qquad j \in C \qquad (4\text{-}34)$$

Reynolds (Re) and Prandtl (Pr) numbers for process cold streams are given as:

$$\mathrm{Re}_j = \frac{4\rho_j Q_j}{\pi \mathrm{D}_j \mu_j} \qquad j \in C \qquad (4\text{-}35)$$

$$\mathrm{Pr}_j = \frac{C_{p,j}\mu_j}{\zeta_j} \qquad j \in C \qquad (4\text{-}36)$$

The heat transfer coefficients h_j can then be estimated by the Equation:

$$h_j = \frac{N_{u,j}\zeta_j}{D_j} \qquad j \in C \qquad (4\text{-}37)$$

Then, the values of h can be fitted to a 2nd order polynomial to predict its value at any temperature for a particular stream as follows:

$$h = \alpha + \beta T + \gamma T^2 \qquad (4\text{-}38)$$

This variability in h will impact the calculations of areas in equations 4-39, 4-40 and 4-41 since h was a constant in the formulation presented in chapter 3. Equation 4-38 provides the means to introduce the effects of heat capacity, viscosity and thermal conductivity profiles into the design of heat exchangers within the superstructure and ultimately, the optimum HEN.

9. <u>Contact area for matches, i,j, i,CU, HU,j in stage k:</u>

$$A_{ijk} = \left(\frac{q_{ijk}}{\left[(dt_{ijk})(dt_{ijk+1}) \left(\frac{dt_{ijk} + dt_{ijk+1}}{2} \right) \right]^{\frac{1}{3}}} \right) \times \left(\frac{1}{h_i} + \frac{1}{h_j} \right), i \in H\ ,\ j \in C\ ,\ k \in K, \quad (4\text{-}39)$$

$$A_{i,CU} = \left(\frac{q_{i,CU}}{\left[\left(dt_{CU,i}\right)\left(T_i^T - T_{CU}^S\right) \left(\frac{dt_{i,CU} + T_i^T - T_{CU}^S}{2} \right) \right]^{\frac{1}{3}}} \right) \times \left(\frac{1}{h_i} + \frac{1}{h_j} \right),\ i \in H \qquad (4\text{-}40)$$

$$A_{HU,j} = \left(\frac{q_{HU,j}}{\left[\left(dt_{HU,j}\right)\left(T_{HU}^S - T_j^T\right) \left(\frac{dt_{HU,j} + T_{HU}^S - T_j^T}{2} \right) \right]^{\frac{1}{3}}} \right) \times \left(\frac{1}{h_i} + \frac{1}{h_j} \right),\ j \in C \qquad (4\text{-}41)$$

Note that the $LMTD_{ijk}$ in above equations is calculated using the Chen approximation (1987).

10. <u>Objective function:</u>

$$\min \sum_{i\in H} CCUq_{i,CU} + \sum_{j\in C} CHUq_{HU,j} + \sum_{i\in H}\sum_{j\in C}\sum_{k\in K} CF_{i,j} C_{p_{i,j}} z_{ijk} + \sum_{i\in H} CF_{i,CU} C_{p_{i,CU}} z_{i,CU}$$

$$+\sum_{j\in C} CF_{HU,j} C_{pHU,j} z_{HU,j} + \sum_{i\in H}\sum_{j\in C}\sum_{k\in K} C_{i,j}\left(A_{ijk}\right)^{\lambda_{ij}} + \sum_{i\in H} C_{i,CU}\left(A_{i,CU}\right)^{\lambda_{i,CU}}$$

$$+\sum_{j\in C} C_{HU,j}\left(A_{HU,j}\right)^{\lambda_{HU,j}} \qquad (4\text{-}42)$$

4.5 Results and Discussions

The same case studies in chapter 3 will be utilized in our analysis for this chapter. In this section, we will introduce more facts about these case studies that pertain to our newly developed formulation in section 4.4. As a reminder, the data for viscosity, heat capacity and thermal conductivity were sourced from ASPEN HYSYS unless otherwise disclaimed.

4.5.1 Case Study 1

The stream data for this case study is presented in table 4-2. The heat capacity correlations for each species can be found in section 3.5.1. Other stream properties and the curve fittings for *h* are also covered below.

The flow rate for all streams in this case study were assumed to be 200 L/min, except for sodium hydroxide which was 1000 L/min. This was done mainly to keep *Re* in the designated range (see section 4.4). For the base case, values of heat capacity, viscosity, thermal conductivity and heat transfer coefficient were estimated at the supply temperatures.

Table 4-2: Stream data for case study 1

Stream	***Compound***	T^S ***(K)***	T^T ***(K)***	***F (kg/s)***
H1	Water	368	318	3.33
H2	Sodium Acetate	353	313	5.10
C1	Ethyl Acetate	293	363	2.99
C2	Sodium Hydroxide	298	398	4.17
HU	Steam	680	680	-
CU	Cooling Water	300	320	-

Table 4-3: stream properties for water in case 1.

T [K]	ζ [W/m.K]	μ [Pa.s]	Cp [kJ/kg K]	Re	Pr	Nu	h [kW/m^2 K]
293	0.5991	1.02E-03	4.185	79175	7.13	344.0	3.925
298	0.6063	9.13E-04	4.185	88589	6.30	362.6	4.187
303	0.6132	8.20E-04	4.185	98630	5.59	381.3	4.453
313	0.6259	6.71E-04	4.185	120455	4.49	418.8	4.992
323	0.6374	5.60E-04	4.185	144456	3.67	456.1	5.537
333	0.6477	4.74E-04	4.185	170471	3.06	493.1	6.083
343	0.6567	4.08E-04	4.185	198228	2.60	529.5	6.623
353	0.6645	3.55E-04	4.185	227455	2.24	565.2	7.154
363	0.6710	3.14E-04	4.185	257855	1.96	600.1	7.669
372	0.6759	2.83E-04	4.185	286049	1.75	630.6	8.119

Table 4-4: Stream properties for sodium acetate.

T [K]	ζ [W/m.K]	μ [Pa.s]	Cp [kJ/kg K]	Re	Pr	Nu	h [kW/m^2 K]
293	0.1394	1.77E-05	2.811	6983705	0.357	5044.8	13.395
298	0.1377	1.77E-05	2.832	6983705	0.364	5074.7	13.310
303	0.1360	1.77E-05	2.854	6983705	0.372	5105.5	13.225
313	0.1325	1.77E-05	2.897	6983705	0.387	5168.7	13.044
323	0.1289	1.77E-05	2.939	6983705	0.404	5234.1	12.851
333	0.1253	1.77E-05	2.982	6983705	0.421	5301.9	12.653
343	0.1216	1.77E-05	3.025	6983705	0.441	5372.8	12.444
353	0.1178	1.77E-05	3.067	6983705	0.461	5446.7	12.221
363	0.1139	1.77E-05	3.11	6983705	0.484	5525.0	11.986
372	0.1104	1.77E-05	3.148	6983705	0.505	5597.3	11.770

Table 4-5: Stream properties for ethyl acetate.

T [K]	ζ [W/m.K]	μ [Pa.s]	Cp [kJ/kg K]	Re	Pr	Nu	h [kW/m^2 K]
293	0.1457	4.55E-04	1.905	314225	5.945	1172.7	6.413
298	0.1439	4.30E-04	1.924	332043	5.753	1209.6	6.533
303	0.1421	4.08E-04	1.942	350621	5.569	1247.1	6.651
313	0.1385	3.66E-04	1.974	390058	5.221	1323.5	6.880
323	0.135	3.30E-04	2.002	432833	4.895	1401.8	7.103
333	0.1314	2.98E-04	2.025	478814	4.599	1482.2	7.310
343	0.1278	2.70E-04	2.044	528395	4.325	1564.9	7.506
350	0.1253	2.53E-04	2.055	565182	4.146	1623.8	7.636

Table 4-6: Stream properties for sodium hydroxide

T [K]	ζ [W/m.K]	μ [Pa.s]	Cp [kJ/kg K]	Re	Pr	Nu	h [kW/m^2 K]
293	0.5235	3.45E-01	2.184	2883	1440.564	247.1873	4.857
298	0.5297	3.00E-01	2.184	3324	1234.865	260.4358	5.177
303	0.5359	2.61E-01	2.183	3813	1063.596	273.8014	5.507
313	0.5483	2.01E-01	2.182	4953	799.894	301.1803	6.198
323	0.5607	1.57E-01	2.181	6333	611.474	329.2755	6.929
333	0.5731	1.25E-01	2.180	7977	474.723	357.9109	7.698
343	0.5855	1.01E-01	2.179	9906	374.021	386.8976	8.502
353	0.5979	8.18E-02	2.178	12166	298.086	416.4636	9.345
363	0.6103	6.74E-02	2.176	14766	240.383	446.1707	10.219
372	0.6215	5.71E-02	2.175	17423	199.967	473.1529	11.036

Table 4-7: Curve fitting coefficients for h (case 1).

Species	Water	Sodium Acetate	Ethyl acetate	NaOH
α	-1.41E+01	1.37E+01	-1.22	2.06
β	6.78E-02	1.41E-02	2.95E-02	-4.46E-02
γ	-2.00E-05	-5.21E-05	-1.15E-05	1.85E-04

The results of applying the formulation on the case study are provided below in the form of tables and figures. Heating loads and exchanger areas in the superstructure can be found in tables 4-8 and 4-9. Also, the interval temperatures for process streams are shown in table 4-10. A cost comparison between the base case and the variable case is displayed in table 4-11 and figure 4-3. Finally, a summary of results is provided in the form of diagrams in figures 4-4 and 4-5.

By analyzing the costs associated with the process, heating and cooling utilities have changed by -2.1% and 24.8%, respectively. By comparing these results with the ones from section 3.5.1, we can conclude that the added stream property profiles have no effect on utility costs. This is due to the fact that only heat capacity is involved in the energy balances that dictate the utility requirements.

Looking at the fixed costs, we observe an increase by 43.4% compared to the base case. Conversely, the results from chapter 3 show a slight increase in this category by 4.4% due to the involvement of variable heat capacity in the calculation of Prandtl number, while keeping other properties constant. For this chapter, allowing the other properties to vary has caused a significant jump in costs, since properties are changing in the superstructure from right to left. Ultimately, this has caused an increase in predicted minimum TAC by 3.4%.

Table 4-8: Results for base case.

Match (i,j,k)	1,2,2	2,2,2	CU,1	CU,2	HU,1	HU,2
q (kW)	530.1	359.7	167.4	265.9	399.0	3659.2
Area (m^2)	4.134	2.936	13.813	25.156	0.405	4.489

Table 4-9: Results for modified case.

Match (i,j,k)	1,2,2	2,2,2	CU,1	CU,2	HU,1	HU,2
q (kW)	529.6	525.1	167.2	373.3	576.0	3398.9
Area (m^2)	3.68	3.781	14.55	35.151	0.535	2.918

Table 4-10: Stage interval temperatures (K) (case 1).

Base Case	**k=1**	**k=2**	**k=3**	**Var. properties**	**k=1**	**k=2**	**k=3**
H1	368	368	330	**H1**	368	368	330
H2	353	353	330	**H2**	353	353	330
C1	293	293	293	**C1**	293	293	293
C2	317.6	317.651	298	**C2**	321.6	321.6	298

Table 4-11: Cost comparisons for case 1.

Base Case	Cost ($/yr)	Var. Prop.	Cost ($/yr)
Heating utility	324654	**Heating utility**	317991
Cooling utility	6499	**Cooling utility**	8108
Fixed costs	40640	**Fixed costs**	58284
TAC	371794	**TAC**	384383

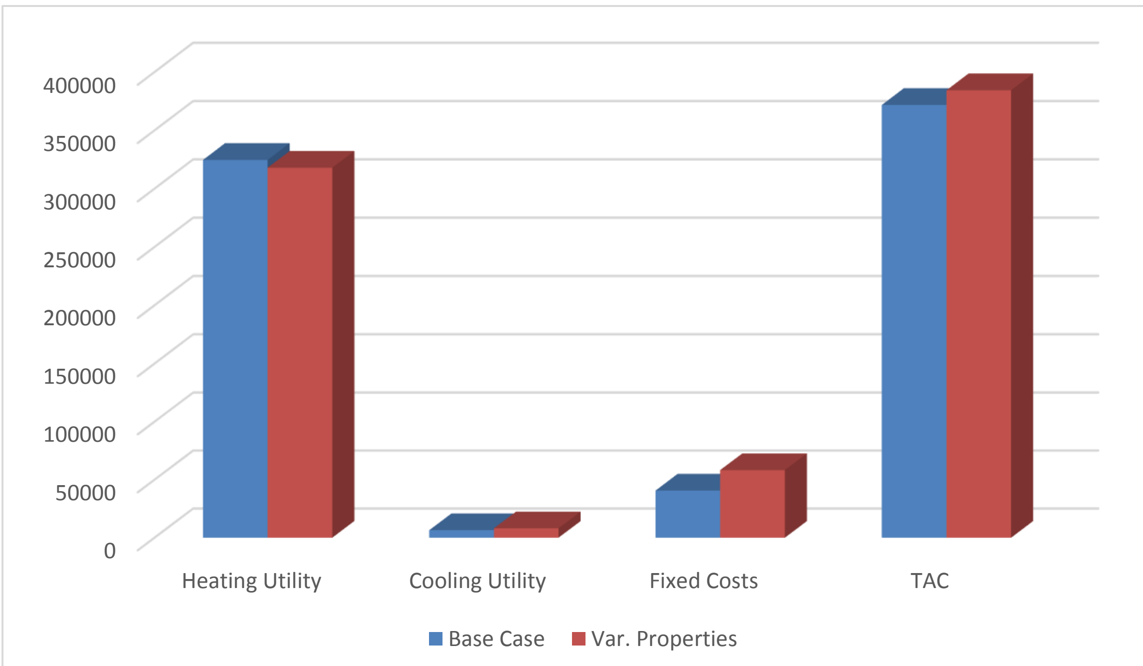

Figure 4-3: Cost Comparisons for case study 1

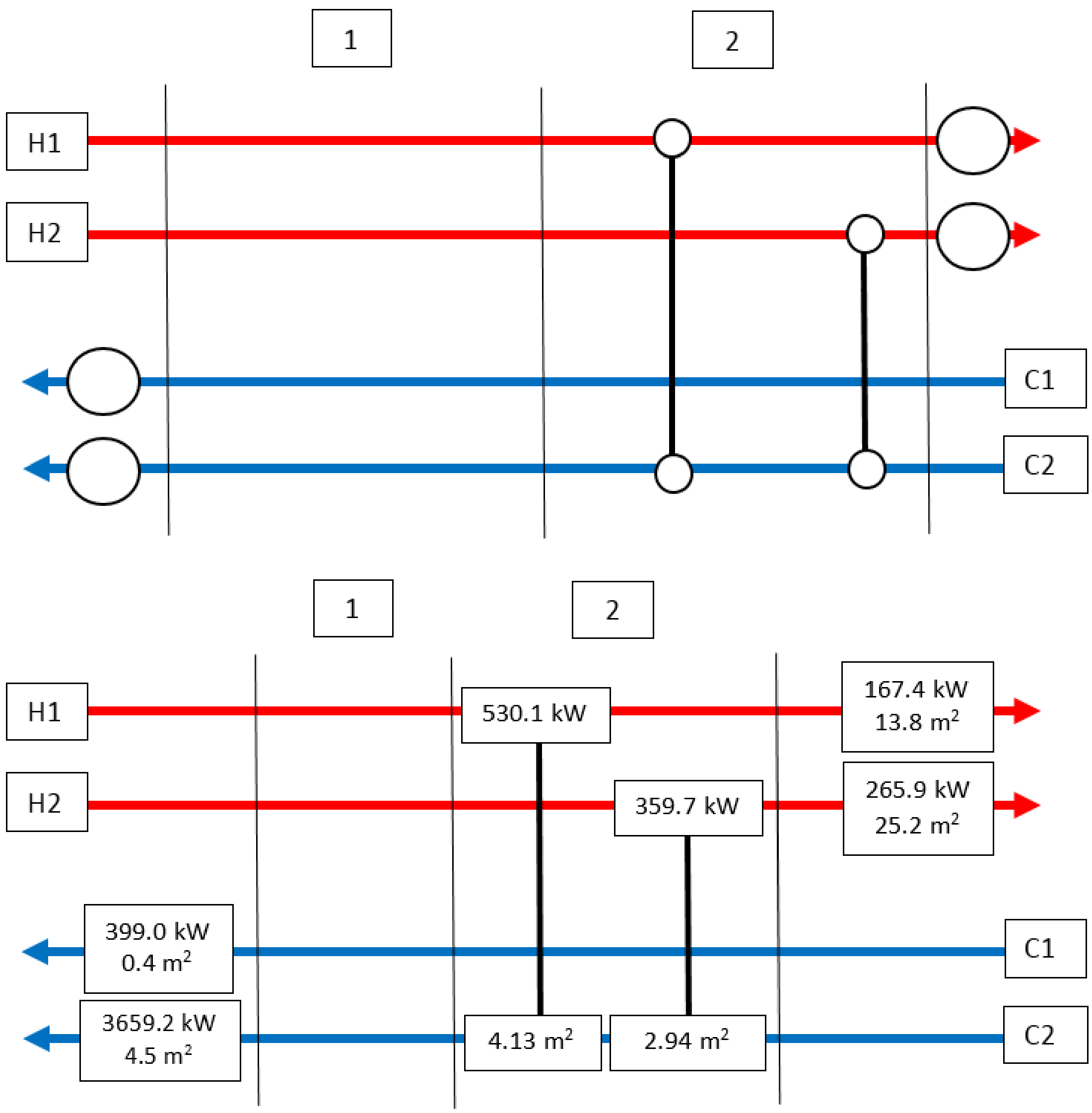

Figure 4-4: Graphical summary of base case 1.

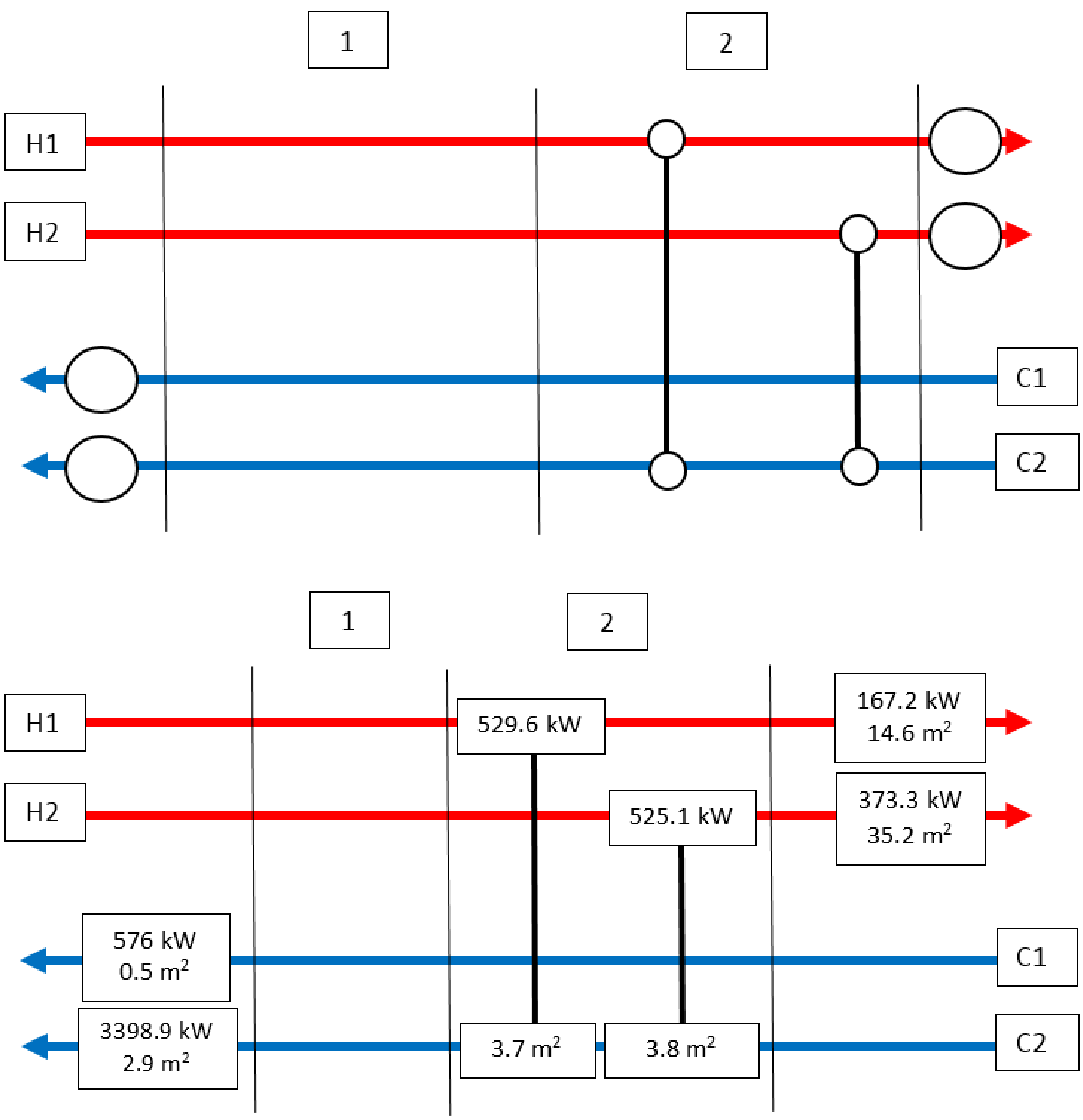

Figure 4-5: Graphical summary of variable properties case 1.

4.5.2 Case Study 2

The stream data for this case study is presented in table 4-12. The heat capacity correlations for each species can be found in section 3.5.2. Other stream properties and the curve fittings for *h* are also covered below.

The flow rate for all streams in this case study were assumed to be 200 L/min, which was done mainly to keep *Re* in the designated range (see section 4.4). For the base case, values of heat capacity, viscosity, thermal conductivity and heat transfer coefficient were estimated at the supply temperatures. Similar to case study 1, cold streams flow in the inner tube (1-inch, schedule 40), while hot streams flow in the outer tube (2-inch, schedule 40).

Table 4-12: Stream data for case study 2

Stream	Compound	T^S (K)	T^T (K)	F (kg/s)
H1	Ethyl benzene	358	313	2.89
H2	Styrene	348	308	3.03
C1	Benzene	303	348	2.92
C2	Water	308	323	3.33
HU	Steam	680	680	-
CU	Cooling Water	300	320	-

Table 4-13: Stream properties for ethyl benzene.

T [K]	ζ [W/m.K]	μ [Pa.s]	Cp [kJ/kg K]	Re	Pr	Nu	h [kW/m^2 K]
293	0.1301	6.77E-04	1.664	103541	8.653	451.8164	1.120
298	0.1289	6.35E-04	1.690	110256	8.329	469.7143	1.153
303	0.1277	5.98E-04	1.716	117133	8.036	487.7311	1.186
313	0.1253	5.33E-04	1.768	131418	7.521	524.2384	1.251
323	0.1229	4.79E-04	1.821	146355	7.091	561.4023	1.314
333	0.1205	4.33E-04	1.874	161881	6.729	599.0656	1.375
343	0.1182	3.94E-04	1.927	177916	6.418	636.9857	1.434
353	0.1158	3.60E-04	1.981	194463	6.162	675.6379	1.490
363	0.1134	3.31E-04	2.035	211427	5.945	714.6737	1.544
373	0.1110	3.06E-04	2.088	228833	5.758	754.0909	1.594

Table 4-14: Stream properties for styrene.

T [K]	ζ [W/m.K]	μ [Pa.s]	Cp [kJ/kg K]	Re	Pr	Nu	h [kW/m^2 K]
293	0.1376	7.54E-04	1.662	97520	9.10	437.3	1.146
298	0.1365	7.01E-04	1.684	104839	8.65	456.3	1.186
303	0.1354	6.54E-04	1.705	112374	8.23	475.3	1.226
313	0.1332	5.74E-04	1.750	128105	7.54	514.0	1.304
323	0.1310	5.08E-04	1.795	144620	6.96	553.0	1.380
333	0.1288	4.54E-04	1.841	161817	6.49	592.4	1.453
343	0.1266	4.09E-04	1.888	179617	6.10	632.2	1.524
353	0.1244	3.71E-04	1.936	197956	5.78	672.2	1.593
363	0.1222	3.39E-04	1.984	216695	5.51	712.3	1.658
373	0.1200	3.12E-04	2.033	235744	5.28	752.5	1.720

Table 4-15: Stream properties for benzene.

T [K]	ζ [W/m.K]	μ [Pa.s]	Cp [kJ/kg K]	Re	Pr	Nu	h [kW/m^2 K]
293	0.1448	0.000639	1.671	218350	7.379	955.5	5.193
298	0.1433	0.0006	1.679	232804	7.026	986.3	5.305
303	0.1418	0.000563	1.723	247892	6.843	1026.2	5.461
308	0.1402	0.00053	1.750	263569	6.612	1063.1	5.594
313	0.1387	0.000499	1.777	279953	6.389	1100.5	5.728
323	0.1356	0.000444	1.833	314656	5.998	1178.1	5.996
333	0.1326	0.000396	1.890	352202	5.650	1258.9	6.265
343	0.1295	0.000356	1.948	392501	5.351	1343.3	6.529
348	0.1280	0.000337	1.978	413790	5.214	1386.8	6.662
353	0.1265	0.00032	2.008	435745	5.086	1431.1	6.794

Table 4-16: Stream properties for water in case 2.

T [K]	ζ [W/m.K]	μ [Pa.s]	Cp [kJ/kg K]	Re	Pr	Nu	h [kW/m^2 K]
293	0.5991	1.02E-03	4.185	156008	7.13	720.3	16.196
298	0.6063	9.13E-04	4.185	174558	6.30	749.9	17.063
303	0.6132	8.20E-04	4.185	194344	5.59	779.2	17.933
313	0.6259	6.71E-04	4.185	237348	4.49	837.2	19.666
323	0.6374	5.60E-04	4.185	284640	3.67	893.8	21.381
333	0.6477	4.74E-04	4.185	335901	3.06	948.9	23.066
343	0.6567	4.08E-04	4.185	390594	2.60	1002.3	24.704
353	0.6645	3.55E-04	4.185	448183	2.24	1054.0	26.287
363	0.6710	3.14E-04	4.185	508084	1.96	1104.0	27.801
372	0.6759	2.83E-04	4.185	563639	1.75	1147.4	29.106

Table 4-17: Curve fitting coefficients for h (case 2).

Species	Ethyl Benzene	Styrene	Benzene	Water
α	-1.86	-2.36	-3.50	-5.50E+01
β	1.35E-02	1.57E-02	3.20E-02	3.05E-01
γ	-1.14E-05	-1.28E-05	-7.99E-06	-2.12E-04

The mathematical formulation in this chapter was applied to case study 2 (see table 4-12) and results were obtained in the same manner as case study 1. Similar sets of results are provided in tables 4-18 to 4-21 and figure 4-4 has a cost comparison for the base case and the variable case. Finally, figures 4-7 and 4-8 summarize the results graphically.

The hot and cold utility costs have changed from the base case by -1.3% and 46.2%, respectively. If we compare these changes to the ones found in chapter 3, we observe that utility costs have changed slightly, unlike in case study 1. This is due to the fact that adding variability to h caused the PTP heat exchanges to decrease by 1, causing stage matches and heating requirements to change slightly.

In a similar manner to case study 1, the fixed costs have increased compared to the base case by 6.9%. These costs have led to a minimum TAC that is higher by 7.2%. Contrasting these results with ones from chapter 3, we can see that adding variability to properties associated with h can be impactful on the optimum HEN.

Table 4-18: Results for base case.

Match (i,j,k)	1,1,1	2,1,2	CU,1	CU,2	HU,2
q (kW)	157.820	68.530	103.180	163.07	209.25
Area (m^2)	11.115	1.753	14.434	23.074	0.145

Table 4-19: Results for Variable case.

Match (i,j,k)	1,1,2	2,2,2	CU,1	CU,2	HU,1	HU,2
q (kW)	303.773	187.644	173.365	215.804	184.993	21.604
Area (m^2)	9.35	5.33	27.146	42.881	0.19	0.015

Table 4-20: Stage interval temperatures (K) (case 2).

Base Case	**k=1**	**k=2**	**k=3**	**Var. Properties**	**k=1**	**k=2**	**k=3**
H1	358	330.79	330.79	**H1**	358	358	330.1
H2	348	348	336.164	**H2**	348	348	330.1
C1	348	316.624	303	**C1**	331.83	331.831	303
C2	308	308	308	**C2**	321.451	321.451	308

Table 4-21: Cost comparisons for case study 2.

Base Case	Cost ($/yr)	Var. Properties	Cost ($/yr)
Heating utility	16740	**Heating utility**	16528
Cooling utility	3994	**Cooling utility**	5838
Fixed costs	62578	**Fixed costs**	66906
TAC	83312	**TAC**	89272

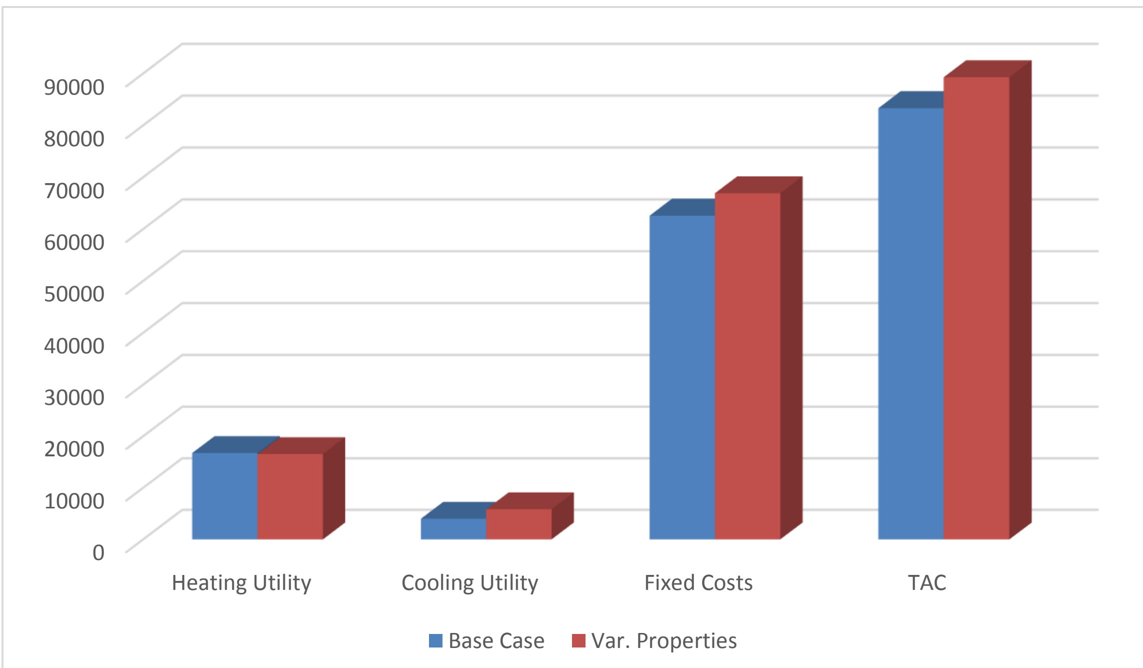

Figure 4-6: Cost Comparisons for case study 2.

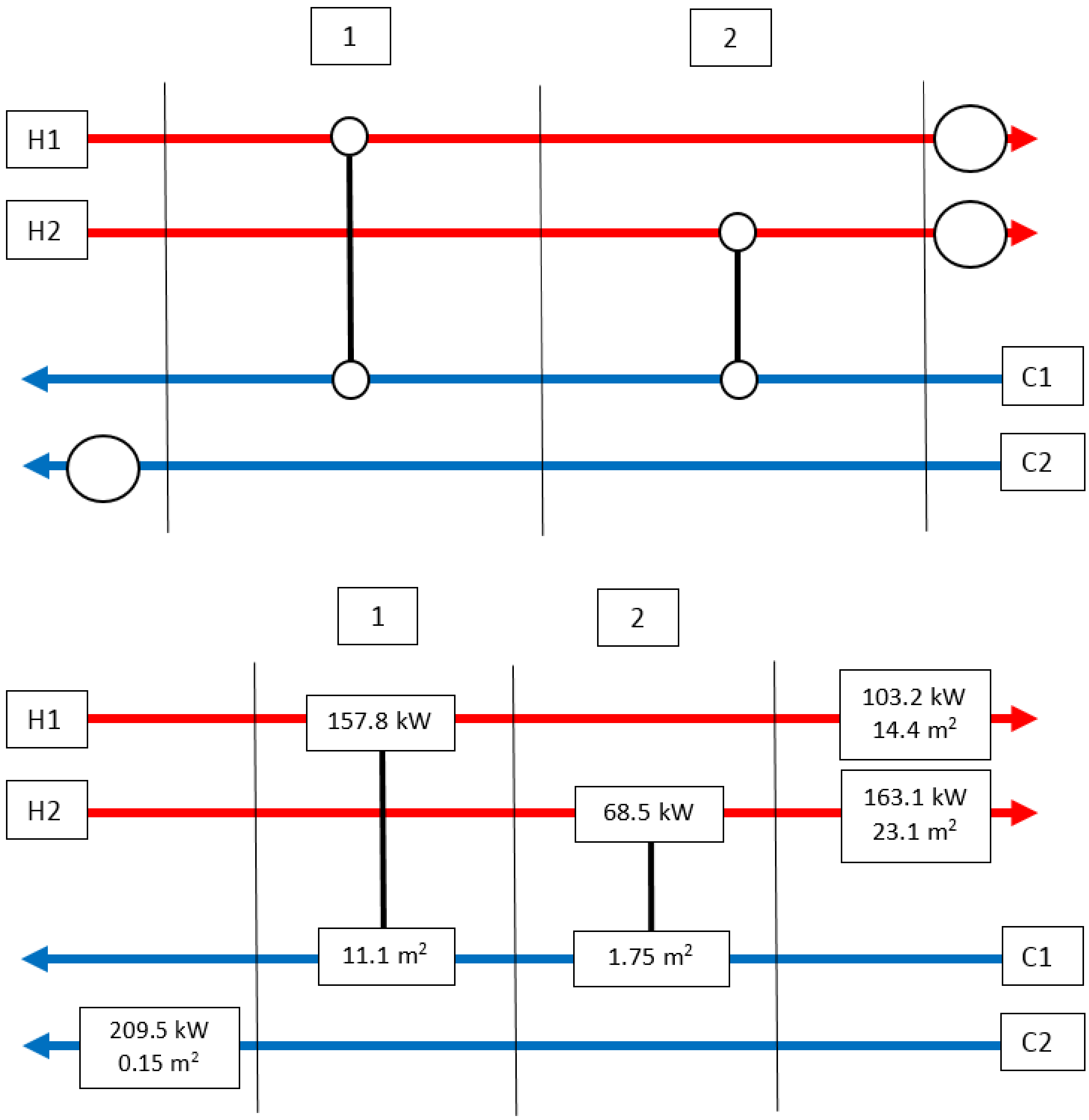

Figure 4-7: Graphical summary of base case 2.

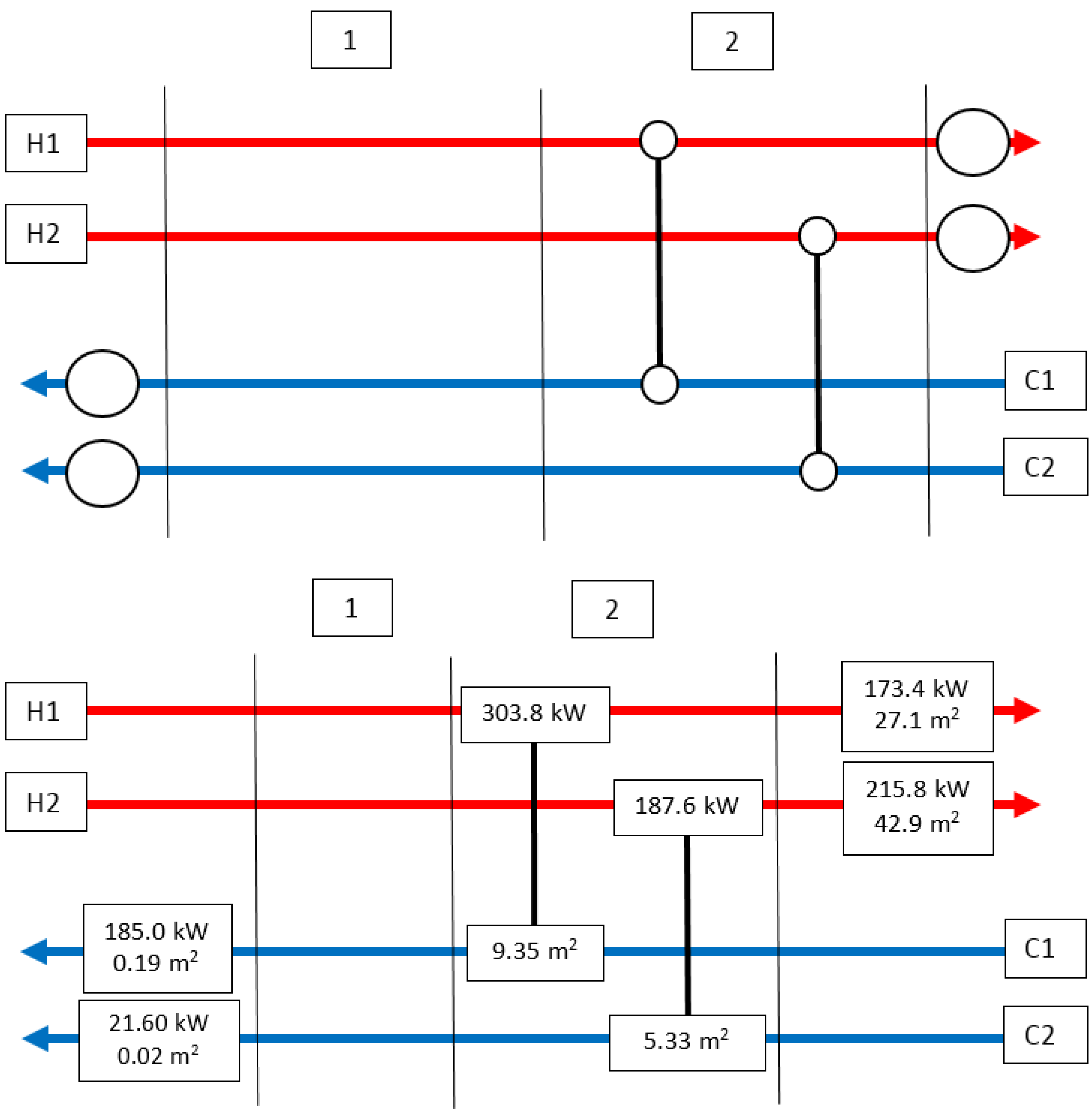

Figure 4-8: Graphical summary of variable properties case 2.

CHAPTER 5

CONCLUSIONS AND RECOMMENDATIONS

The effects of stream property profiles on process optimization were investigated. This was done by modifying an established mathematical formulation to account for variability in those properties. First, variable heat capacity was introduced to a newly developed model. Then, after getting results from two different case studies, another mathematical formulation was attempted to account for other stream properties. This was done by including variable terms for viscosity, thermal conductivity and heat transfer coefficient. Next, the latest formulation was applied to the same case studies and the results were analyzed.

The minimum TAC in these case studies has changed in the range of -0.9% to 7.2% compared to base cases (where properties are assumed constant). It was also observed that fixed costs are mostly affected by heat exchanger design variables (h, μ and ζ) while utility costs are mostly affected by variable heat capacity.

These results are comparable to recent efforts in this field. In their work, *Nejad et al.* [27] have concluded that the pinch point for the ammonia plant in their research has increased by 3 ^{o}C, and hot and cold utilities load has increased by 23% and 11%, respectively. Additionally, the area of the heat exchanger network has increased by 50%. As discussed earlier in the literature review, their conclusions were based on a graphical method based on stream segmentation.

In other work we already cited in chapter 2, Al-Mutairi and Odejobi [30] have introduced variable capacity flow rate (FC_p) on the optimization of HEN in a thermal power plant. They used an MINLP optimization model by comparing a base case with two cases involving the same thermal plant with a 5% increase and a 5% decrease in capacity flow rate, respectively. An increase of 5% caused a 4.4% rise in heating load and 3.9% increase in cooling load. On the other hand, a decrease of 5% resulted in a heating load reduction of 4.9% and a cooling load decrease of 4.9%. Results from these efforts show that introducing variable physical properties can have a significant outcome on the optimization of HENs.

These efforts look at the process and the variability of its properties through macro-level factors. By changing our perspective to micro-level factors, as we did in this research, and allowing stream properties to directly vary as a function of temperature, we can come closer to accurately predicting the optimum HEN, especially when done using mathematical programming.

In the industry, classic mathematical formulations have done an adequate job in synthesizing optimal networks. However, the results on paper can markedly differ from the actual application. For instance, an optimum HEN on paper that promises a 20% reduction in utility costs would reduce costs in the actual process by 15% or less. Our work is designed to provide decision makers in the industry better, more sophisticated tools that bridge the gap between theory and reality.

We can look at the measurement of time as a good analogy. In the past, people measured time using primitive means, such as the hourglass, which gave them a general idea about time durations. On the other hand, we now have the tools to measure time accurately and to the millisecond. The novel formulations developed in this research are a worthy step into improving the tools of process optimization.

In the future, it is recommended that other factors should be investigated to provide even more improvements to optimization tools. For instance, we should look at the impact of non-pure streams on optimality as well as the existence of phases other than liquid, such as non-ideal gas mixtures, in process streams. Another factor that should be examined is the heat exchanger configuration. We could look at changing the configuration to other types, such as shell-and-tube or cross-flow, and see how that can impact the flow regime and the optimum HEN. We can also look at the effects of exertion and fouling on the heat exchangers and provide a real-time simulation of how the optimum HEN and the heat loads are affected by these aforementioned factors.

Nomenclature

Indices

i hot process stream

j cold process stream

k index for stages (k = 1,…, NOK), and temperature location (k = 1,…, NOK+1)

CU cold utility

HU hot utility

Sets

H $\{i \mid i$ is a hot process stream$\}$

C $\{j \mid j$ is a cold process stream$\}$

K $\{k \mid k$ is a stage in the superstructure, $k = 1,\ldots, NOK\}$

Parameters

T_i^S supply temperature of hot stream i

T_{HU}^S supply temperature of hot utility

T_i^T target temperature of hot stream i

T_j^S supply temperature of cold stream j

T_{CU}^S supply temperature of cold utility

T_j^T target temperature of cold stream j

ΔT_{min} minimum approach temperature

F_i mass flow rate of hot stream i

F_j mass flow rate of cold stream j

A_i contact area for hot stream

A_j contact area for cold stream

ζ thermal conductivity

Q volumetric flow rate

$U_{i,j}$ overall heat transfer coefficient for hot stream i and cold stream j

CCU cost per unit of cold utility

CHU cost per unit of hot utility

CF fixed charge for exchangers

h stream heat transfer coefficient

C area cost coefficient

C_p heat capacity

a, b, c species-dependant heat capacity coefficients

D diameter of pipe

NOK total number of intervals

λ area cost index

Ω an upper bound for heat exchange

μ viscosity

α, β, γ species-dependent *h* coefficients

Γ an upper bound for temperature difference in match ij

N_u Nusselt number

Re Reynolds number

Pr Prandtl number

<u>Binary Variables</u>

z_{ijk} variable indicating the existence of match ij in interval k in optimal network

$z_{i,CU}$ variable indicating the existence of match between hot stream i and cold utility

$z_{HU,j}$ variable indicating the existence of match between hot utility and cold stream j

<u>Variables</u>

dt_{ijk} driving force for match ij in interval k

$dt_{i,CU}$ temperature approach for the match of hot stream i and cold utility

$dt_{HU,j}$ temperature approach for the match of hot utility and cold stream j

q_{ijk} heat exchanged between hot stream i and cold stream j in temperature interval k

$q_{i,CU}$ heat exchanged between hot stream i and cold utility

$q_{HU,j}$ heat exchanged between hot utility and cold stream j

$t_{i,k}$ temperature of hot stream i at hot end of interval k

$t_{j,k}$ temperature of cold stream j at hot end of interval k

References

1. S.A. Papoulias and I.E. Grossmann, *A Structural Optimization Approach in Process Synthesis--II: Heat Recovery Networks.* Computers & Chemical Engineering, 1983. **7**(6): p. 707-721.

2. S.A. Papoulias and I.E. Grossmann, *A Structural Optimization Approach in Process Synthesis--I: Utility Systems.* Computers & Chemical Engineering, 1983. **7**(6): p. 695-706.

3. S.A. Papoulias and I.E. Grossmann, *A Structural Optimization Approach in Process Synthesis--III: Total Processing Systems.* Computers & Chemical Engineering, 1983. **7**(6): p. 723-734.

4. M.A. Duran and I.E. Grossmann, *Simultaneous Optimization and Heat Integration of Chemical Processes.* AIChE Journal, 1986. **32**(1): p. 123-138.

5. I.E. Grossmann, H. Yeomans and Z. Kravanja, *A Rigorous Disjunctive Optimization Model for Simultaneous Flowsheet Optimization and Heat Integration.* Computers & Chemical Engineering, 1998. **22**(Supplement 1): p. S157-S164.

6. K.L. Yee and N. Shah, *Improving the Efficiency of Discrete Time Scheduling Formulation.* Computers & Chemical Engineering, 1998. **22**(Supplement 1): p. S403-S410.

7. T.F. Yee and I.E. Grossmann, *Simultaneous Optimization Models for Heat Integration--II. Heat Exchanger Network Synthesis*. Computers & Chemical Engineering, 1990. **14**(10): p. 1165-1184.

8. T.F. Yee, I.E. Grossmann and Z. Kravanja, *Simultaneous Optimization Models for Heat Integration--III. Process and Heat Exchanger Network Optimization*. Computers & Chemical Engineering, 1990. **14**(11): p. 1185-1200.

9. E.N Pistikopoulos and I.E. Grossmann, *Optimal Retrofit Design for Improving Process Flexibility in Nonlinear Systems--II. Optimal Level of Flexibility*. Computers & Chemical Engineering, 1989. **13**(10): p. 1087-1096.

10. M.M. El-Halwagi, *Process Integration*. First edition. 2006, San Diego, CA: ELSEVIER Inc.

11. R. Smith, *Chemical Process Design and Integration*. 2005, Chichester, England: John Wiled & Sons Ltd.

12. M.A. Duran and I.E. Grossmann, *Simultaneous Optimization and Heat Integration of Chemical Processes*. 1986. p. 123-138.

13. C.L. Chen and P.S. Hung, *Simultaneous Synthesis of Flexible Heat-Exchange Networks with Uncertain Source-Stream Temperatures and Flow Rates*. Industrial & Engineering Chemistry Research, 2004. **43**(18): p. 5916-5928.

14. C.L. Chen and P.S. Hung, *Synthesis of Flexible Heat Exchange Networks and Mass Exchange Networks.* Computers & Chemical Engineering, 2007. **31**(12): p. 1619-1632.

15. H. Rodera, D.L. Westphalen and H.K. Shethna, A *Methodology for Improving Heat Exchanger Network Operation.* Applied Thermal Engineering, 2003. **23**(14): p. 1729-1741.

16. J. Zhang and X.X. Zhu, *Simultaneous Optimization Approach for Heat Exchanger Network Retrofit with Process Changes.* Industrial & Engineering Chemistry Research, 2000. **39**(12): p. 4963-4973.

17. K.P. Papalexandri, D.I. Patsiatzis, E.N. Pistikopoulos and L. Ebbesen, *Heat Integration Aspects in a Crude Preheat Refinery Section.* Computers & Chemical Engineering, 1998. **22**(Supplement 1): p. S141-S148.

18. R. Adonyi, J. Romero, L. Puigjaner and F. Friedler, *Incorporating Heat Integration in Batch Process Scheduling.* Applied Thermal Engineering, 2003. **23**(14): p. 1743-1762.

19. E.M. Al-Mutairi and M.M. El-Halwagi, *Incorporation of Scheduling Considerations in Retrofitting Design of Heat Exchange Networks.* Chemical Engineering Transactions, 2009. **18**: p. 421-429.

20. N. Zhang and W. Verheyen, *Design of Flexible Heat Exchanger Network for Multi-Period Operation.* Chemical Engineering Science, 2006. **61**(23): p. 7730-7753.

21. H.G. Dong, C.Y. Lin and C.T. Chang, *Simultaneous Optimization Approach for Integrated Water-Allocation and Heat-Exchange Networks.* Chemical Engineering Science, 2008. **63**(14): p. 3664-3678.

22. H.G. Dong, C.Y. Lin and C.T. Chang, *Simultaneous Optimization Strategy for Synthesizing Heat Exchanger Networks with Multi-Stream Mixers.* Chemical Engineering Research and Design, 2008. **86**(3): p. 299-309.

23. K.C. Furman and N.V. Sahinidis, *A Critical Review and Annotated Bibliography for Heat Exchanger Network Synthesis in the 20th Century*. Industrial & Engineering Chemistry Research, 2002. **41**(10): p. 2335-2370.

24. A. Querzoli, A. Hoadley and T. Dyson, *Identification of Heat Integration Retrofit Opportunities for Crude Distillation and Residue Cracking Units*. Korean Journal of Chemical Engineering, 2003. **20**(4): p. 635-641.

25. D.M. Fraser and N.E. Gillespie, *The Application of Pinch Technology to Retrofit Energy Integration of an Entire Oil Refinery*. Chemical engineering research & design, 1992. **70**(A4): p. 395-406.

26. B. Al-Riyami, J. Kelmes and S. Perry, *Heat Integration Retrofit Analysis of a Heat Exchanger Network of a Fluid Catalytic Cracking Plant.* Applied Thermal Engineering, 2001. **21**: p. 1449-1487.

27. S.H.A. Nejad, F. Shahraki, M.R.S. Birjandi, A. Kovac Kralj and F. Fazlollahi, *Modification of Heat Exchanger Network Design by Considering Physical Properties Variation.* Chem. Biochem. Eng. Q. 2012. **26**: p. 79-87.

28. A.J. Isafiade and D.M. Fraser, *Interval Based MINLP Superstructure Synthesis of Heat Exchanger Networks for Multi-Period Operations.* Chemical engineering research & design, 2010. p. 1329-1341.

29. M.M. Faruque Hasan, Iftekhar A. Karimi and Hassan E. Alfadala, *Synthesis of Heat Exchanger Networks Involving Phase Changes.* Proceedings of the 1st Annual Gas Processing Symposium. 2009. p. 185-192.

30. E. Al-Mutairi and O. Odejobi, *Investigating the Thermodynamics and Economics of Operating the Thermal Power Plant under Uncertain Conditions.* Energy Conversion and Management. 2013. **75**: p. 325-335

31. R. Felder and R. Rousseau, *Elementary Principles of Chemical Processes.* 3rd edition; Wiley, 2000.

32. J.P. Holman, *Heat Transfer.* 9th edition; McGraw-Hill, 2002.

33. R. Bird, W. Stewart and E. Lightfoot, *Transfer Phenomena.* 2nd edition; Wiley, 2007.

34. R. Reid, J. Prausnitz and B. Poling, *The Properties of Gases and Liquids.* 4th edition; McGraw-Hill, 2004.

35. J. Wilkes, *Fluid Mechanics for Chemical Engineers*. 2nd edition; Prentice-Hall, 2006.

Vitae

Name	Faysal Mohammad Al Khulaifi
Nationality	Saudi
Date of Birth	4/16/1987
Email	khulaifi87@gmail.com
Address	Dhahran, Saudi Arabia

Academic Background

M.Sc., Chemical Engineering, (2014)

King Fahd University of Petroleum and Minerals

Dhahran, Saudi Arabia

B.Sc., Chemical Engineering, (2011)

King Fahd University of Petroleum and Minerals

Dhahran, Saudi Arabia